Appendixes

Substances Whose Production or Environmental Release Are Likely to Increase in the Next 10 Years*

by Clement Associates, Inc.

OTA requested Clement Associates to develop a list identifying new chemical substances likely to be manufactured in the near future and known chemicals likely to pose an increased burden to the environment because of increased production, new applications, or new technological developments, including new energy technology. For these projections, several factors were considered, including market trends, Federal regulatory activity, available substitutes for recently banned or restricted chemical substances, and consumer needs.

During the development of the approach to this phase of the project, certain problems and limitations became apparent. The nature of chemical substances under research and development but not yet introduced to the market is usually closely guarded proprietary information and therefore not available. In addition, there are no data systems which bring together chemical information to facilitate the retrieval of necessary data. An approach was developed to obtain a maximum amount of information in a limited amount of time.

Sources, including personal contacts, were identified for information on new chemicals or chemicals whose production, use, and release to the environment were likely to increase sharply because of future needs. These sources of information are listed in the reference list.

Following are the list of chemicals and a brief indication of why these chemicals were selected.

CHEMICALS LIKELY TO HAVE SIGNIFICANTLY GREATER ENVIRONMENTAL RELEASE IN THE NEAR FUTURE

Chemicals Whose Production and Use Are Likely to Increase Sharply Because of Future Needs

Soluble Polymers

Soluble polymer "completing" agents are being developed to remove toxic metals from waste waters or remove radioactive metals from nuclear waste fluids. Polyethylene glycol *and its* derivatives are the most versatile of the soluble polymers. Others are polyethyleneimine, polyvinyl sulfonic acid, polyacrylic acid with such chelating groups as thiourea, 8-hydroxyquinoline, iminodiacetic acid and hydroxyciniline, and polymers based on acrylic acid. (C&EN, Mar. 27, 1978, p. 24)

Organic Flocculants

The principal organic flocculants are polyacrylamides, polyamides, and polyepichlorohydrins. Stiffening waste treatment regulations to reduce sludge are making flocculants more attractive. The chemicals make up a $100 million per year

*Excerpt from OTA Working Paper entitled "Priority Setting of Toxic Substances for Guiding Monitoring Programs. " A complete copy of the paper can be obtained through the National Technical Information Service. (See app. J.)

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market that may double within the next 5 years. These polymers may also be used for enhanced oil recovery if the price of oil would rise to make enhanced recovery economical. (C&EN, Jan. 23, 1978, p. 9)

Multifunctional Acryiates

The use of radiation curing (ultraviolet or electron beam) is rapidly increasing. Radiation curing contributes significantly to critical energy savings and pollution abatement. Demand for the following multifunctional acrylates used for ultraviolet inks and coatings is expected to increase: pentaerythritol triacrylate, 1,6-hexanedioldiacrylate, trimethylolpropane triacrylate, and tetraethylene glycol. (C&En, Jan. 23, 1978, p. 12, Celanese Chemical Co. Advertisement)

Polyester Resin

Concern about energy will augment the growth of lightweight polyester resin in the United States through the 1980's. The need for lighter weight materials in the automotive market, as well as the demand for corrosion-resistant products in many areas, will increase the demand for polyester resin at an average of 9.2 percent a year through 1987. Polybutylene terephthalate (PBT) and polyethylene terephthalate (PET) will be among the fastest growing polyester resins. PBT and PET are expected to grow from a combined demand of 38 million lbs in 1977 to 322 million lbs by 1987—an average annual growth rate of 24 percent. PBT is currently the most widely used thermoplastic polyester resin. However, it is expected that PET production will increase more rapidly, overtaking PBT production. The total polyester resin market is expected to rise 140 percent in the next 10 years. other uses and average annual projected production increases from 1977 to 1987 include unsaturated reinforced polyester (9. 1 percent), thermoset surface coatings (5 percent), cultured marble and other unsaturated thermoses (4.0 percent), strapping (mostly scrap, 28 percent), and fibers (4.0 percent). (C&EN Jan. 30, 1978, p. 11)

Zeolites

Zeolites (aluminosilicates) hold promise as detergent builders, A 25-million-lb market in 1977 has a prospect of a possible 400-million-lb market in 1982. Zeolites containing detergents perform "equivalent or roughly equivalent" to the phosphate-silicate formulations that now command 75 percent of the current heavy-duty powder market. Environmental problems will continue to push phosphate out of the heavy-duty home laundry market. Zeolite 4A is a cubic crystalline sodium aluminosilicate with the formula

$$Na_2 \cdot Al_2O_3 \cdot 2SiO_2 \cdot 45H_2O.$$

Textile Chemicals

The market for textile chemicals is expected to top the billion-dollar market by 1980. Examples are:

Chemical	Use
Biphenyl	Dye bath additives
o-phenylphenol	
1,2,4-trichlorobenzene	
Methyl naphthalene	
Perchloroethylene	
Alkyl aryl sulfonic acids	
Ethoxylated alcohols	
Quaternary ammonium compounds	
Ethoxylated nonyl phenol	
Alcohols of alkyl aryl sulfonic acid	
Esters of phosphoric acid	
Acrylic latex	Finishing agents
Styrene-butadiene rubber latex	
Polyvinyl alcohol	
Polyvinyl acetate	
Melamine formaldehyde	
Starches	
Polyvinylchloride	
Fluorochemicals	
Glyoxal (dimethylol, dihydroxyethylene urea)	
Carbamate (isobutyl, 2-methoxyethyl)	
Tetrakis phosphonium sulfate 'ammonia	
Cyclic phosphonates	
Maleic anhydride	Printing chemicals
Polyacrylic acids	
Acrylates	
Butadiene acrylonitrile	
Hexamethylol melamine formaldehyde	
Dioctyl sulfosuccinates	
Ethoxylates	
Pentachlorophenon	Bacteriocides
o-phenylphenol	
Low C_H and aromatic distillates	
Urea	
Ethoxylated alkyl phenols	[dispersing agents/mulsifiers
Sodium lauryl sulfate	

(C&EN, May 29, 1978, p. 12)

Pumice

Pumice has many similarities with asbestos. They are both mineral oxides, low in density, heat resistant, nonflammable, chemically inert, and low in cost, Rhodes (Division of Beatrice Foods Co., Des Plains, Ill.) claims pumice may be the safe and economical alternative to asbestos (C&EN, May 22, 1978, p. 9). The manufacturer suggests that pumice be used in paints; chemicals (filtration media and chemical carrier); leather buffing: compounders (powdered hand soaps and glass cleaners); metal and plastic finishing; and applacations in the dental, rubber, glass, furniture, electronics, and pottery industries.

Polyvinylacetates

Acrylic and acetate resins compete in the market as textile and binder emulsions for nonwoven fabrics. Currently, acrylics dominate both of these markets by two-thirds of the total, Polyvinylacetates make up only 14 percent of the market, with the remainder going to other resins. New technical developments may change the status quo. By 1987, acetates could surpass acrylics in many quality paint and textile markets. (C&EN, Mar, 20, 1978, p. 11)

Hydrazine and Its Derivatives

Originally used in rocket fuels, today hydrazine and its derivatives are commercially used in herbicides, pesticides, blowing agents for plastics, and water treatments. Its consumption is growing by 15 percent per year according to Olin Chemicals' advertisement in C&EN.

Olefinic Thermoplastic Elastomers

Olefinic thermoplastic elastomers are also called TPO rubbers and were introduced in 1973, having a market volume of 1.5 million lbs. It is anticipated that the demand for TPO rubber will reach 44 million lbs by 1980 and that uses in automobiles will account for more than half of it. Mechanical goods and wire and cable uses account for 12.7 and 18,2 percent of TPO demand, respectively. Olefinic thermoplastic elastomers are also used by carmakers in electrostatically paintable body filler panels, air deflectors, and stone shields. Recently they have been used as sound deadening material on diesel-powered vehicles, jacketing and insulating material for wire and cable coating, and many custom-molded and extruded mechanical goods. (C&EN, Oct. 23, 1978, p. 9)

Silicones

New markets for silicones as PCB replacements in electrical transformers, in brake fluids, and as elastomers are developing. Methylchloride is used as an intermediate in the production of silicones, Other methylating agents could be used to replace methyl chloride in most applications, but the potential substitutes (e.g., dimethyl sulfate, methyl bromide, methyl iodide) are much more expensive and have toxicity and handling problems which make them less desirable.

Chlorobromination

Bromine chloride has been shown to be more effective as a disinfectant than chlorine in field trials. It is a heavy red liquid and 12 times more soluble in water than chlorine. Its vapor pressure is one-third as great. Bromine chloride completely hydrolyzes almost immediately to hypobromous acid and reacts with ammonia in sewage to form bromoamines. It is believed that chlorobromination is the best alternative to current chlorination practices.

Polyethyleneterephthalate

DuPont is continuing a vigorous effort to develop a market for molded plastics made from conventional forms of thermoplastic polyethylene terephthalate. (See also Polyester resin,) This resin has a multibillion-pound demand as polyester fibers and films and is finding a large market in plastic beverage bottles. DuPont's trade name for PET is Rynite. Rynite's prime targets will be metals replacement, especially in automobiles.

Chemicals Produced or Released Due to Energy Development Technology

Coal Liquefication and Gasification Program

The conversion of coal to liquid to gaseous hydrocarbons for fuel technologies will result in the release of many chemicals to the environment. The contaminants may enter the environment via two pathways: 1) emission into the atmosphere with the consequent potential for long-range transport and 2) direct discharge via runoff and leaching into the aquatic and terrestrial domain where impact might be expected to be more localized. Contaminants from coal combustion can be classified into three groups: 1) organic chemicals, 2) inorganic chemicals, and 3) radionuclides.

Organic Contaminants

Organic contaminants from coal-derived process can be placed into several categories as shown below.

Category	*Example*
Acids and anhydrides	Maleic anhydride
	Benzoic acid
Amines	Aniline
	Alpha and beta naphthylamines
	Methylaniline
	Benzidine
Carbonyl compounds	Formaldehyde
	Acetaldehyde

Hetrocyclics	Pyridines
	Quinolines
Simple aromatic hydrocarbons ., ., ...	Benzene
	Toluene
	Xylenes
Phenols.	Phenols
	Cresols
	Xylanols
Polycyclic aromatic hydrocarbons	Benzo(a)pyrene
	Dibenzofluorene
	Dibenzoanthracene
	Benzoanthracenes
	Benzo(a)anthrone
	Dimethylbenzoanthracene
	Chrysene
	Methylchrysenes
	Benzocarbozoles
	Idenopyrenes
	Carbozoles
	Pyrenes
	Biphenyl
	Acenapthalene
	Acenapthalyne
	Fluorene
	Alkylanthracenes
	Alkylphenanthracenes
	Anthracene
	Perylene
	Benzoperylene
	Coronene
Sulfur compounds	Thiophenes
	Mercaptans
	Carbon disulfide
	Methyl thiphene
Organometallics. , ., . . .,	Nickel carbonyl
	Tetraethyl lead
Naphthyl cyanides ,. . . .,	Napthyl cyanide
	Ammonium thiocyanate

Trapped organic compounds and aromatic units in coals that were isolated, separated, and identified by gas chromatography and mass spectrometry are shown in table A-1.

Inorganic Chemicals

Category	Examples	
Acids	Sulfuric acid	
	Nitric acid	
	Hydrochloric acid	
Chromium salts	Chromium chloride	
	Chromium sulfide	
Sulfur compounds	Hydrogen sulfide	
	Carbon disulfide	
Trace elements. . . . , ,	Antimony	Manganese
	Arsenic	Mercury
	Barium	Molybdenum
	Beryllium	Nickel
	Bismuth	Selenium
	Cadmium	Silver
	Chromium	Tellurium
	Cobalt	Thallium
	Copper	Tin
	Fluorine	Uranium
	Gallium	Vanadium
	Lead	Zinc

Fine particulate , ...	Sulfur particulate
	Respirable coal dusts
	Tar
	soots
Gasses	Carbon monoxide
	Sulfur dioxide
	Sulfur trioxide
	Sulfur tetraoxide
	Nitrous oxide

Radionuciides

Emissions from a 100-MW electricity generation powerplant that burns coal at a rate of approximately 100 tons per hour are estimated to contain 1 ppm of uranium and 2 ppm of thorium, A plant of this size is expected to release 1 percent of its fly ash to the atmosphere. Under these conditions thorium-228 and -232, radium-224, and lead-212 each contribute approximately 5 x 10^{-3} Ci per year; uranium-234 and -238, thorium-230 and -234, radium-226, lead-210, polonium-210, and bismuth-2 10 each contribute approximately 8 x 10^{-3} Ci per year; uranium-235 and praseodymium-231 both contribute approximately 3.5 x 10^{-4} Ci per year; and radon-220 and -222 together account for approximately 1.2 Ci per year. (ERDA report 77-64, August 1976)

Radioactive emissions of bituminous coals have a high uranium content (75 ppm).

Solar Heating and Cooling of Buildings

Water contamination can occur in solar-heated domestic hot water systems at heat exchanger interfaces. Serious health consequences could be expected if the contaminated water is ingested. Water contamination could result from the heat exchange fluids themselves, or in water-based systems from such additives as:

Corrosion inhibitors—Chromates, berates, nitrates, nitrites, sulfates, sulfites, arsenates, benzoate salts, various triazoles, silicates, and phosphate compounds.

Freeze protestants—Glycols.

Heat transfer fluids—Paraffins, aromatic and other synthetic hydrocarbons.

Bacteriacides— Chlorinated phenols.

Solar collectors used in heating and cooling systems utilize organic chemical compounds as insulators that can emit highly toxic substances under overheat or fire conditions. Fumes usually consist of simple starches and phenolic compounds: ammonia, hydrochloric acid, hydrofluoric acid, toluene diisocyanate (TOI), and hydrogen cyanide.

Table A-1.—Trapped Organic Compounds and Aromatic Units in Coal

1. Straight-chain hexane
2. 2-hexene
3. Dimethylbutane, methylcyclopentane
4. cyclohexane
5. C_7-alkene (B)
6. Benzene
7. Thiophene
8. C_7-alkane (B), C_7-alkene (B)
9. C_7-alkadiene (B) or c_7-alkyne (B)
10. Cyclohexene
11. C_7-alkane (B)
12. Dimethylcyclopentane
13. 2- and 3-methylhexanes
14. Heptene
15. 2,3-dimethyl-2-pentene
16. Methylcyclohexane
17. Dimethylhexane
18. Heptyne
19. Trimethylpentane
20. Methylheptane
21. Methylheptene
22. Trimethylcyclopentane
23. 1-methylcyclohexene
24. Toluene
25. Dimethylcyclohexane
26. Methylthiophene
27. C_9-alkene (B)
28. Ethylcyclohexane
29. Trimethylcyclohexane
30. *n*-propyl and/or isopropylcyclohexane
31. C_3-alkylcyclopentane (?)
32. C_9-alkane (B), C_9-alkene
33. C_9-alkyne (?) and/or C_9-alkadiene (?)
34. Ethylbenzene
35. Dimethylthiophene
36. *m*, and *p*-xylene
37. *o*-xylene
38. C_9-alkene (B)
39. tetramethylcyclohexane
40. C_{10}-alkene (B)
41. C_3-alkylcyclohexane
42. Diethylcyclohexane (?)
43. C_{10}-alkane (B), C_{10}-alkene (B)
44. C_{10}-alkene
45 Ethyloctane (?)
46 Trimethylthiophene
47 Propylbenzene
48 Methyl ethylbenzene
49 Trimethylbenzene
50 C_{11}-alkene (B)
51 C_4-alkylbenzene
52. C_{11}-alkene (B) and C_4-alkylbenzene
53 Tetramethylbenzene
54 1-methyl-4-isopropyl-3-cyclohexene (?)
55 Methylindan
56 C_{12}-alkene (B)
57 Dimethylindan
58 C_5-alkylbenzene
59 Tetralin
60 C_5-alkylbenzene
61. C_{13}-alkene, C_6-alkylbenzene
62 Naphthalene
63 C_{13}-alkane (B), C_{14}-alkene (B)
64 2-methylnaphthalene
65 1-methylnaphthalene
66 C_1-alkyldecalin
67 C_4-alkyldecalin
68 Trimethylindan
69 Tetramethylindan and/or trimethyltetralin
70 C_9-alkylcyclohexane
71 Biphenylene
72 2-ethylnaphthalene
73 1-ethylnaphthalene
74 Dimethylnaphthalene
75 Cadinane (4,10-dimethyl-7-isopropyldecalin)
76 Dihydrocadinene (T), C_9-alkylcyclohexane
77 Selinane and eremophilane (hydronaphthalenes)
78 Dihydroselinene (T) and/or dihydroeremophilene (T)
79 Dihydrocadinene (T)
80 C_5-alkylindan
81 Methylcenaphthene, 2(?)-isopropylnaphthalene
82 Diphenylmethane
83 3 or 4-methylbiphenyl
84 C_{10}-alkylbenzene
85 Tetramethylindan
86 $C_{15}H_{28}$-sesquiterpenoid hydrocarbon (?)
87 C_5-alkyltetralin
88 Methyl-ethylnaphthalene and/or trimethylnaphthalene
89 Trimethylnaphthalene
90 Fluorene
91 1,6-dimethyl-4-isopropyl-1, 2-dihydronaphthalene (T)
92 Iso-butylnaphthalene, trimethylnaphthalene
93 1-methyl-4-isopropyl-naphthalene
94 Eudalene (1-methyl-7-isopropyl-naphthalene)
95 C_5-alkyltetralin (?)
96 1-methyl-2-propylnaphthalene (T)
97 Cadalene (1,6-dimethyl-4-isopropyl-naphthalene)
98 Tetramethylnaphthalene
99. 1,4-dimethyl-6 (?)-isopropyl-naphthalene, C_6-alkyltetralin (T)
100 C_6-alkyltetralin (T)
101 1,2,5,7-tetramethyl-naphthalene
102 Pristane
103 Methylfluorene
104 Pentamethylnaphthalene
105 Dibenzothiophene
106 Trimethyloctahydro-phenanthrene
107 Methyltetrahydrophenanthrene (T)
108 Phenanthrene
109. $C_{14}H_{23}$ (*m/e* 191, base peak), $C_{20}H_{16}$ (M^+) tricyclic terpenoid (?)
110. Dimethyltetrahydrophenanthrene (T)
111. Ethyltetrahydrophenanthrene (T)
112. Anthracene
113. Naphthofuran
114. Methyldibenzothiophene
115. C_9-alkyltetralin (?)
116. $C_{20}H_{32}$ (abietadiene (?))
117. $C_{10}H_{10}$ (tricyclicditerpenoid (?))
118. 2- and/or 3- methylphenanthrene
119. 1- and/or 9-methylphenanthrene
120. 1,7-dimethylphenanthrene
121. Dimethyldibenzothiophene
122. C_{10}-alkyltetralin (or C_{11}-alkylindan) (?)
123. Dehydroabietene (4,20-dimethyl-13-isopropyl-8H-phenanthrene)
124. Dimethylphenanthrene and/or dimethylanthracene
125. Dehydroabietane
126. $C_{20}H_{12}$ (tricyclic-diterpenoid) (?)
127. Fluoranthene
128. C_{11}-alkyltetralin (?)
129. Abietatetraene (T) (trimethylisopropyl-6H-phenanthrene)
130. 1,2,3,4-tetrahydroretene (T)
131. Methyl-ethylphenanthrene and/or trimethylphenanthrene
132. Pyrene
133. Simonellite
134. Retene (1-methyl-7-isopropylphenanthrene)
135. 1,2-benzofluorene
136. 2,3-benzofluorene
137. 3,4-benzofluorene
138. Methylpropylphenanthrene and/or dimethylethylphenanthrene
139. Methylbenzofluorene
140. Tetramethylphenanthrene and/or tetramethylanthracene
141. Chrysene and/or triphenylene

B = branched T = identification tentative ? = identification uncertain

Fuels From Biomass

Thermochemical biomass conversion can produce gases, tars, oils, and unconverted residue (char) and ash, depending on the particular conversion process. Thermochemical reactions generated sulfur-containing (H_2S, COS, CS_2, SOX) and nitrogen-containing (HCN, NOX, NH_3) gases.

Water can be affected by the residuals produced from thermochemical conversion. Low-molecular weight oils, phenols, leachates from char and ash residues, and scrubber solution runoff may enter water bodies by direct discharge or by percolation to subsurface waters from evaporation points.

REFERENCE LIST FOR SUBSTANCES WHOSE PRODUCTION OR ENVIRONMENTAL RELEASE ARE LIKELY TO INCREASE IN THE NEXT 10 YEARS

Chemical Marketing and Economics Abstracts. The Division of Chemical Marketing and Economics of the American Chemical Society (ACS) presents papers at ACS national meetings on subjects related to the responses of the chemical industry to economic changes as well as responses of the financial community to changes in the chemical industry. Abstracts of these papers are published by ACS.

A Study of Industrial Data on Candidates for Testing. This document, published by the U.S. Environmental Protection Agency, Office of Toxic Substances (EPA Contract No. 68-01-4109, November 1976) contains market forecasts for 10 major classes of chemicals (109 individual chemicals) with an annual production greater than or equal to 1 million lbs. Chemicals that are used exclusively as drugs or pesticides are not included. The market forecasts include: 1) a discussion of production and trade statistics, 2) consumption patterns, whenever possible, 3) growth trends, 4) a brief summary of current uses as well as potential new applications, and 5) growth trends in end-market consumption. A discussion of possible substitutes for some of the chemicals is also included.

Environmental Development Plans. The Environmental Development Plans (EDPs) published by the U.S. Department of Energy (March 1978) were conceived and prepared as basic documents to assist in planning and managing environmental programs of energy technology development. Approximately 30 EDPs covering major developing energy technologies were prepared.

A Review of Current Information on Some Ecological and Health-Related Aspects to the Release of Trace Metals Into the Environment Associated With the Combustion of Coal. This document by Merrill Heit is a technical report (HASL-320) from the Health and Safety Laboratory, Energy Research and Development Administration, New York, N.Y. 10014, reviewing the literature on one class of pollutants. Information on the environmental levels, ecological effects, and potential toxicity to man of 35 elements that may be released into the environment by coal combustion or gasification is presented.

Fossil Energy Update. This monthly journal compiled by the Department of Energy lists abstracts of current scientific and technical reports, journal articles, conference proceedings, theses, and monographs on all aspects of fossil energy, including factors involving the environment, health, and safety.

Chemical Engineering News. The Chemical Engineering News is a weekly publication of the American Chemical Society that contains relevant information in such sections as "Chemical World," "This Week," "Business Concentrates," and "Science/Technology," and in profiles on selected chemicals.

Chemical Marketing Reporter. This weekly, published by Schnell Publishing Company, Inc., contains information on chemical market reports and profiles on selected chemicals.

Trapped Organic Compounds and Aromatic Units in Coal. This article, published by Tyoichi Hayatsu et al. in Fuel 57:541 (1978), contains a detailed analysis of the organic constituents of three coals: a lignite, a bituminous, and an anthracite. Organic compounds trapped in the coal matrix, residuals, and products of the original coalification process were described.

Personal Communications With Several Organizations, Including the Chemical Development Association and Chemical Marketing Research Association.