Health and Environmental Effects Document for Direct Coal Liquefaction - 1981

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HEALTH AND ENVIRONMENTAL EFFECTS DOCUMENT FOR
DIRECT COAL LIQUEFACTION - 1981

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1.0 SUMMARY

This document presents initial estimates of potential human health effects from inhalation of nonmethane hydrocarbons (NMHC) that may be released from a future hypothetical industry producing about 600,000 bbl/day of synthetic fuel by direct liquefaction of coal. The assessment approach starts with general assumptions that are then refined in a tiered sequence that considers available epidemiological, environmental and chemical data. The uncertainties involved in such an evaluation have been quantified where possible at this early stage of health risk analysis.

Many surrogate data bases were considered for application to coal liquefaction including coke oven, British gas retort, roofing tar and asphalts, and cigarette smoke. The coke oven data base was selected for this assessment because the chemical and physical nature of coke oven emissions are judged to more closely approximate potential coal liquefaction emissions.

Utilizing the extensive epidemiological data base for coke oven workers as a surrogate model, health effects from release of coal liquefaction NMHC may be quantified. This method results in estimates of about 1×10^{-3} excess cancer deaths/yr to the industrial work force of 7800 persons and 5×10^{-2} excess cancer deaths/yr in the U.S. population as a whole from NMHC that boil above 600°F.

Sources of uncertainty in the estimates include: the rate of release of high-boiling NMHC (2.4 to 21.6 g/sec); the magnitude of occupational exposures (2.4×10^5 to 4.2×10^6 person-ng/m³) and east central public exposures (9.5×10^6 to 1.7×10^8 person-ng/m³) resulting from release; the carcinogenic potency of high-boiling NMHC is assumed to be the same as the potency of coke oven emissions. Using these uncertainties, it is estimated that from 2×10^{-4} to 5×10^{-3} lung cancer deaths/yr may occur in the industrial work force and from 1×10^{-2} to 2.5×10^{-1} lung cancer deaths/yr in the U.S. population as a whole. On an individual basis, the excess lifetime risk to occupationally exposed workers is estimated to be 500 times greater than to members of the U.S. public.

2.0 INTRODUCTION

U.S. reliance on foreign oil products has stimulated interest in alternative methods of producing clean gaseous, liquid, and solid fuels. Coal and oil shale are primary sources of such "synthetic" fuels. Both coal and oil shale can be converted into a variety of fuels that could replace many natural gas and petroleum products.

Human health and environmental effects of developing energy technologies must be assessed to assure the establishment of environmentally acceptable technologies. The procedure by which these effects are analyzed is necessarily iterative. The purpose of this document is to provide a rudimentary and an analytical approach illustrating how the potential health risk, in terms of one exposure pathway--inhalation of nonmethane hydrocarbons (NMHC) released from a hypothetical commercialized coal liquefaction industry can be quantified. The initial analysis is limited in terms of scope of source terms considered, environmental pathways, and human health endpoints, as characterized by the term "zero order." It examines the occupational and public health effects that may result from inhalation of high-boiling nonmethane hydrocarbons released from a future hypothetical direct coal liquefaction industry (DOE 1981a). It should be noted that we assume the high boiling point NMHC (>600°F) emissions will act as aerosols in the ambient air and thus only small particle transport was modeled. No commercial coal liquefaction facility presently exists in the U.S. The data base for assessment was derived from pilot plant operation and related industrial experience. A principal objective of chemical and biological characterization of SRC-II pilot plant samples at the Pacific Northwest Laboratory (PNL) has been to use results to assess health and environmental impacts of commercial scale coal liquefaction facilities (Weimer et al. 1980).

Certain hydrocarbons have long been suspected as contributors to carcinogenicity in humans. A wide range of NMHC are produced and released to the environment from conventional coal utilization processes. Epidemiological

studies, ongoing for several decades, of workers employed in these processes, indicate that prolonged exposure to the NMHC in coal-derived liquid volatiles, coke oven emissions, coal tar products and asphalt fumes can result in increased rates of skin, lung, scrotal and other organ cancers. However, the specific chemical components of NMHC responsible for the increased risk to humans have not been identified and a dose-response relationship relative to specific chemicals has not been established. It should also be noted that during the pilot phase of current U.S. efforts (1973-1981) to develop direct coal liquefaction processes, no occupational cancers have been reported. This may be due to increased attention to worker hygiene or to insufficient time for most organ cancers to develop because of their long latency period. In a coal hydrogenation plant at Institute, West Virginia, Sexton (1960) reported cutaneous cancers and precancerous lesions in workers exposed to coal liquefaction products. In a recent follow-up mortality study of the workers with skin cancer and precancerous lesions, no cancer deaths were observed (Palmer 1974). A mortality study is now underway of the total Institute coal hydrogenation plant work force (according to Dr. Susan Austin, Union Carbide Staff Epidemiologist). Although there are differences between the Institute plant and proposed coal liquefaction plants in exposure levels, this population can provide important insight into potential occupational health risks.

A comprehensive risk assessment requires in-depth consideration of numerous human health and environmental issues. The zero-order assessment reported here is only a preliminary step in such an undertaking, and it is not intended that the assessment even approximate a comprehensive evaluation. A wide range of facility emissions must be considered from each part of any proposed coal utilization process, e.g., mining, plant operation, product transportation, product use, waste disposal. Process characterization has been grossly simplified as a necessary feature of the present analysis; however, such factors will be handled in more detail in future iterations of this document, leading to a more complete assessment.

3.0 PROCESS DESCRIPTION

Direct coal liquefaction processes are generally similar with respect to many of their unit operations. Therefore, this assessment, based on the SRC-II process, may be considered representative of other coal liquefaction processes presently under development. Because the environmental data base for SRC-II is larger than that for other coal liquefaction processes, it was selected for the assessment. A commercial direct coal liquefaction facility would consume about 30,000 tons of coal per stream day (tpsd) while producing about 100,000 bbl/day of liquid product (DOE 1981a).

The SRC-II process converts high-sulfur bituminous coal into low-sulfur, low-ash liquid fuel products; secondary gaseous and liquid products; and by-product sulfur, ammonia, and phenolics. Pulverized and dried coal is mixed in a slurry with a recycled solvent produced in the process and reacted with hydrogen at high temperature and pressure (see Figure 3.1). After separation of gaseous products and unreacted hydrogen, the liquid products are processed to separate the residue (ash and unreacted coal) from the primary and secondary products. Some heavy-end slurry product containing mineral residue is recycled to the process. The remaining mineral-rich residues are processed in a gasifier to produce synthesis gas ($H_2 + CO$). The slag (primarily mineral ash) remaining after gasification is the principal solid waste. Most of the sulfur and part of the nitrogen in the coal react with hydrogen to form hydrogen sulfide and ammonia that are removed from the gaseous products and recovered as by-product elemental sulfur and ammonia.

Transfer operations and transport spills may release coal-derived liquids and vapors to the environment. Volatiles may be released during startup, shutdown, upsets, maintenance and routine operations. Any point in the process where high boiling coal-derived liquids or their vapors escape may be considered a potential hazard. This assessment deals only with high boiling point NMHC released to the atmosphere.

FIGURE 3.1. Schematic of the SRC-II Demonstration Facility Process (PNL 1980)

4.0 NMHC RELEASES TO THE ATMOSPHERE

The major potential sources of all NMHC emissions to the atmosphere include: leaks from valves, flanges, seals, drains; vapors released from storage and loading operations; spills; and venting operations required to prevent overpressuring of process equipment. These emissions can be grouped into fugitive emissions and planned routine atmospheric emissions. The biologically important high-boiling-point emissions (Wilson, Pelroy and Mahlum 1982) make up about 4% of the total NMHC emissions (DOE 1981a). Because there are no operational commercial scale coal liquefaction facilities in the U.S., other industries were examined for possible use as a substitute or surrogate model for coal liquefaction. The petroleum refining industry is often used as a surrogate model for estimating the fugitive and routine emissions from coal liquefaction (NIOSH 1981).

4.1 FUGITIVE EMISSIONS

Fugitive emissions originate from leaks in equipment, mainly valves, flanges, seals, vents, and drains. They are assumed to be ground-level releases, ubiquitously spread throughout the coal liquefaction facility. There are a large number of potential sources, with control typically achieved through a combination of equipment specifications and routine inspection and maintenance. Table 4.1 enumerates these sources for a 6000 ton/day demonstration plant. Actual numbers for a 30,000 ton/day commercial plant would depend on plant configuration and are probably not linearly related but lower. Given the uncertainties regarding plant configuration, we have assumed linear scaling from the demonstration plant to a commercial facility. The NMHC fugitive emissions, based on petroleum refinery operations (EPA 1979) are estimated to be about 2.9 g/s (DOE 1981a). This value multiplied by 5 (i.e., 30,000 tons/day divided by 6,000 tons/day) gives an estimated yield of 15 g/s for a commercial liquefaction facility. Of this emission rate, about 4% (0.6 g/s) (DOE 1981a) is attributed to the biologically active NMHC that boil above 600°F. (Wilson, Pelroy and Mahlum 1982). Only these higher boiling fractions will be considered further.

TABLE 4.1. Number of Possible Fugitive Emission Sources from
a 6000-Ton/Day Demonstration Plant (DOE 1981a)

<u>Plant Unit</u>	<u>Inline Valves</u>	<u>Flanges</u>	<u>Pump Seals</u>	<u>Compressor Seals</u>	<u>Vents and Relief Valves</u>	<u>Open-Ended Valves</u>	<u>Drains</u>
Dissolver	1706	1562	47		12	266	62
Hydrogen Treatment and Recovery	182	128	10	5	6	10	2
Gasifier	380	637	27		7	96	16
Shift Conversion and H ₂ Purification and Compression	155	170	16		1	4	1
∞ Syngas Purification and Methanation	56	60	10		1	4	1
L.P. Gas Treatment	160	215	6	1	1	6	2
Production Gas System	220	315	8	4	3	28	4
Sulfur Recovery	50	70	12		2	10	4
Fractionation	218	300	32		1	59	23
Plant Unit Number	60	95	6	1	2	8	2
Ammonia and Tar Acid Recovery and Oxygen Production	180	215	48		2	16	6
Cooling Tower	230	390	18	2		14	1

4.2 ROUTINE ATMOSPHERIC EMISSIONS

Routine releases of NMHC, primarily from charge heaters, power boiler flue gases and other sources, are identified in Table 4.2. The American Petroleum Institute (API 1973) reported that the largest potential source of hydrocarbon emissions to the atmosphere from a refinery is evaporation loss from tankage. To estimate this loss for coal liquefaction, a definite product must be specified that would be held in storage tanks. This component of routine emissions will be quantified in the next iteration of this document. Information is also not available on emissions from process water treatment. Therefore, these two sources of emissions are not included in this analysis. Multiplying emission values from defined sources by 5, to approximate a commercial scale facility, yields a total routine atmospheric emission of 15 g/s. We assume that routine emissions exhibit the same boiling point characteristics reported for fugitive emissions. Therefore, 0.6 g/s of >600°F materials also applies here and will be considered further.

4.3 CHEMICAL AND PHYSICAL NATURE OF EMISSIONS

Several surrogate data bases were considered for application to coal liquefaction including those for coke oven and British gas retort emissions, as well as roofing-tar and asphalt volatiles, and cigarette smoke (NIOSH 1973, 1977a,b). Criteria considered in the selection of a surrogate included 1) the availability of a suitable epidemiologic data base, 2) data on exposure concentrations, and 3) the comparability of physical and chemical properties to those of potential coal liquefaction emissions. Of the surrogates considered, coke oven emissions best fulfilled these criteria.

In addition to chemical composition, the form in which the various constituents are released into the atmosphere (e.g., aerosols, gases) and the size and density of the particulate matter with which they are associated, determine their effects on human health (EPA 1978). Most of the emitted particles associated with the iron and steel industry, involving

TABLE 4.2. Estimate of Maximum Routine Atmospheric Emissions
at an SRC-II Demonstration Plant (DOE 1981a)

<u>Equipment Name</u>	<u>NMHC Routine Emission(a) Rates (g/s)</u>
Dissolver charge heaters and other proprietary heaters flue gas	0.77
Fractionator reboiler flue gas	0.33
Power boiler flue gas	0.81
Superheater flue gas	0.16
Waste-water incinerator gas	0.03
Oxygen plant fuel gas heater	0.29
Heavy oil product flue gas	0.04
Mineral residue slurry heater	0.04
Thawing shed emissions	0.14
Coal dryer	0.30
SCOT burner and incinerator gas	<u>0.04</u>
	3.0

(a) All release rate numbers have been rounded in this report
to a maximum of two significant figures.

coking, are less than 5 μm before control and probably 90% are fine particles after control (EPA 1981). In addition, the relatively high temperature and high carbon-to-hydrogen ratios of the particulate releases associated with coking operations appear to make these materials a reasonable analogue to potential coal liquefaction NMHC aerosols.

5.0 ATMOSPHERIC DISPERSION

For purposes of atmospheric dispersion modeling, we assume that the biologically active NMHC emissions are all in the form of airborne particulates of respirable size, e.g., $<10\text{ }\mu\text{m}$. From the data presented by the EPA (1981), this appears to be quite realistic. Bioavailability of intercalated organics is not well characterized. However, for respirable particles of less than $2\text{ }\mu\text{m}$, the rate of elution into the lungs of adsorbed PAH's increases with particle size (EPA 1978). Our assumption of 100% bioavailability used in this analysis is undoubtedly an overestimate.

Both near-field and far-field dispersion modeling was used. Near-field modeling predicts the isopleths of ground-level air concentrations within a reference facility site boundary so the potential health effects that may be experienced by occupationally exposed workers can be estimated. The far-field modeling predicts the annual average ground-level air concentrations in the U.S. and multiplies them by the resident population to estimate U.S. public health effects.

5.1 NEAR-FIELD DISPERSION

Routine and fugitive NMHC emissions of $>600^{\circ}\text{F}$ were assumed to originate from the 5 dissolver locations identified within a reference facility site boundary (DOE 1981a) represented by the shaded area of Figure 5.1. Workers who operate and maintain a direct coal liquefaction facility will therefore be exposed to a total of 1.2 g/sec of NMHC emissions. This emission rate was utilized by a sector average Gaussian plume model to compute average annual NMHC concentrations within and surrounding a reference facility site. The results of this modeling effort are shown in Figure 5.1 as isopleths of NMHC above 600°F in units of ng/m^3 . The $130\text{-ng}/\text{m}^3$ isopleth was selected as an average air concentration for the site. Occupationally exposed workers are assumed to inhale air of this concentration.

Near-field dispersion modeling is important to estimate the health risks of airborne NMHC to a population of workers or residents near a coal liquefaction facility. Model details are presented in Appendix A.

FIGURE 5.1. Annual Average Isopleths Overlying a Reference Commercial Coal Liquefaction Facility (ng/m^3)

5.2 FAR-FIELD DISPERSION

Potential health effects that may be experienced by people residing some distance from the sources of NMHC depend not only on pollutant characteristics, but also on meteorological conditions and the geographic distribution of exposed populations. To estimate the U.S. population exposure to airborne NMHC, the total coal liquefaction industry must be considered. The future hypothetical industry scenario consists of 6 commercial (30,000 tpsd coal) facilities, 2 in each of three states--Illinois, Kentucky and West Virginia (DOE 1981a). Each facility is assumed to release 1.2 g/sec of NMHC of $>600^{\circ}\text{F}$ split equally between routine and fugitive sources. This emission rate was utilized by an Air Quality Control Region (AQCR) matrix model (Niemann 1981) and the PNL long-range transport (LRT) model (Eadie and Davis 1979) to determine the combined population exposure to the U.S. public from these 6 commercial coal liquefaction facilities operating together (7.2 g/sec total release).

The AQCR model (discussed in detail in Appendix B) estimates the concentration of respirable particles two meters above ground level in each of the 243 AQCRs produced by a unit of particle emissions from a facility placed in any AQCR. The concentrations in each AQCR are then added for each facility's contribution and isopleths are drawn.

Figure 5.2 shows the concentration isopleths of the combined annual average airborne NMHC emissions from the future hypothetical industry scenario. The results of two additional siting scenarios show the concentration differences expected from varying sites and regional meteorology (see Figures 5.3 and 5.4).

The concentrations of NMHC are then multiplied in the model by the industry work force to obtain a measure of occupational exposure or by the number of people living in each AQCR culminating in person-ng/m³ population exposure values as shown in Table 5.1. These values, now weighted by population density, vary by a factor of three and are used directly in the estimation of potential health effects.

FIGURE 5.2. Future Hypothetical Commercial Coal Liquefaction Facility Locations with Annual Average Isopleths of Airborne NMHC Emissions (ng/m^3)

FIGURE 5.3. Alternative West Coast Siting Scenario with Annual Average Isopleths of Airborne NMHC Emissions (ng/m³) (each asterisk represents 2 facilities)

FIGURE 5.4. Alternative East Coast Siting Scenario with Annual Average Isopleths of Airborne NMHC Emissions (ng/m^3) (each asterisk represents 2 facilities)

TABLE 5.1. Population Exposures

<u>Population</u>	<u>Best Estimate Person-ng/m³(a)</u>	<u>Range Person-ng/m³(b)</u>
Occupational Public	1 x 10 ⁶	2.4 x 10 ⁵ to 4.2 x 10 ⁶
East Central	4 x 10 ⁷	9.5 x 10 ⁶ to 1.7 x 10 ⁸
West Coast	6 x 10 ⁷	1.4 x 10 ⁷ to 2.5 x 10 ⁸
East Coast	2 x 10 ⁷	4.8 x 10 ⁶ to 8.4 x 10 ⁷

(a) All numbers have been rounded to one significant figure.

(b) The range in population exposures is a result of applying the uncertainties of source terms (factor of 3) and dispersion modeling (factor of 3) for a combined uncertainty of about 4.

6.0 HUMAN HEALTH EFFECTS

The present paucity of data make it impossible to accurately relate airborne NMHC concentrations to human carcinogenesis. In 1930 Kenneway and Hieger focused attention on polynuclear aromatic compounds when they produced skin tumors with dibenzanthracene. When Kenneway (1955) isolated benzo(a)pyrene (BaP) from coal tar distillates in 1954, interest shifted to this compound as the determinant carcinogen in coal-derived materials. Many investigators have since used BaP levels in many organic pollutants as an indicator of carcinogenic potential.

Existing PNL information from microbial mutagenesis assays, cultured mammalian cells, and mammal skin painting experiments suggest that with regard to observed genotoxic and carcinogenic effects, higher boiling range SRC materials are of greater concern than those boiling at lower temperatures (Pelroy and Wilson 1981). Most biological activity is observed in materials boiling above about 600°F. In all boiling point cuts, most microbial mutagenesis activity is associated with the nitrogen-containing constituents with the primary aromatic amines being the determinant mutagens. Recent data indicate that PAHs as well as nitrogen-containing compounds are responsible for mammalian cell transformation and skin tumorigenicity activities. Nitrogen-rich fractions from a number of coal-derived hydrocarbon mixtures and pyrolysis products exhibit enhanced mutagenicity compared to the unfractionated source material (Pelroy and Peterson 1979; Ho et al. 1979; and Schuetzel et al. 1982).

This leads to the assumption that only the amount of NMHC in the emission that corresponds to a boiling point in excess of 600°F is of concern relative to tumorigenesis. However, the existence of NMHC that may act as promoters in fractions boiling below 600°F cannot be completely ruled out.

Two approaches are proposed to estimate, as well as possible, potential human health effects from a developing energy technology. The first utilizes coke oven emission and epidemiological data to provide a more reliable basis for deriving health risks. Secondly, it is proposed in Section 6.2 that a matrix be used to statistically test the hypotheses which were derived to

link chemical, biological and epidemiological data. This approach will guide future work, both in research and assessment efforts.

6.1 COKE OVEN WORKER EPIDEMIOLOGICAL DATA

This method utilizes an epidemiologic data base which has a relatively solid foundation. The relatively high temperatures of formation and high carbon-to-hydrogen ratios of the particulates associated with coking operations appear to make these materials a reasonable analogue to potential coal liquefaction aerosols. In addition, coke oven derived creosote oil and SRC-II fuel oil blend have 80 to 85% of their chemical compounds in common, i.e., 2-, 3-, 4-, and 5-ring PAH and their alkyl homologs and heteroatomic derivatives. Therefore, we believe that using epidemiology data from coke ovens as a surrogate for coal liquefaction is reasonable. Exposure levels and tumor incidences are reasonably well documented for coke oven workers. Thus, this data was used for the present assessment.

The rate of elution of PAHs into the lungs increases with increasing particle size from about 0.1 to 2.0 μm (EPA 1978). In the atmosphere of coke ovens, PAHs are primarily found absorbed on particulate matter, which increases the likelihood that PAHs will penetrate into the lungs. Particulates found on top of coke ovens are at the upper end of the respirable particle range and are most significant biologically (EPA 1978).

A recent EPA review of the health effects of coke oven emissions presents data on the temperature range of carbonizing chambers and the excess of lung cancer reported (EPA 1978):

<u>Temperature Range (°F)</u>	<u>Reported Excess of Lung Cancer Among Workers (%)</u>
750 - 932	27
1652 - 2012	83
2192 - 2552	255
<u>> 2732</u>	800

Temperatures reached during the coal liquefaction process will affect the estimated risk of lung cancer.

Particulate levels average about 3 mg/m^3 in work areas (Smith et al. 1979; Redmond et al. 1976; Cuddihy et al. 1980). Lung cancer rates in workers in these areas are about 11 times those for other steel workers or about 4×10^{-3} cancer deaths/yr/worker. This represents an increase of approximately 3.6×10^{-3} cancer deaths/yr/worker above that due to background. Assuming a linear dose-response, 1.2×10^{-3} cancer deaths/yr/person would be expected for a 1 mg/m^3 exposure. This dose-response function is then about 1.2×10^{-9} cancer deaths/yr/person-ng/ m^3 .

Several estimates have been made of lifetime risk of lung cancer associated with exposure to coke oven emissions. Recently, the EPA (1978) calculated that the average lifetime probability of respiratory cancer death due to a lifetime exposure of $1 \text{ } \mu\text{g/m}^3$ of coal-tar-pitch volatiles is 9×10^{-4} . Again assuming a linear dose-response, the value becomes 9×10^{-7} for a lifetime exposure of 1 ng/m^3 . This value is about a factor of 10 higher than the number derived in this study ($1.2 \times 10^{-9} \times 70 = 8.4 \times 10^{-8}$).

6.1.1 Occupational Work Force - Coke Oven Data Model

We assume that the general and administrative personnel mainly occupy ventilated offices and are not exposed to airborne NMHC. Occupationally exposed workers include about 750 plant operating personnel and about 550 maintenance craftsmen (DOE 1981a).

Using the cancer death rate as a function of exposure derived from the coke oven worker data, an additional 1×10^{-3} cancer deaths above background would be expected annually in the coal liquefaction industrial work force of 7800 persons exposed to 130 ng/m^3 . This value translates into an individual risk of about 2×10^{-7} /yr and an excess lifetime probability of dying of respiratory cancer of 1×10^{-5} from this source.

6.1.2 U.S. Population

The additional cancer mortality from the future hypothetical industrial scenario (east central siting) using coke oven emission data as a base amounts to an excess of about 5×10^{-2} deaths/yr in the U.S. population as a whole. By contrast, if all six facilities were sited in California, 7×10^{-2} deaths/yr are estimated due to a larger population living closer to the source; and if the industry was spread along the North and South Carolina coast, less than 2×10^{-2} cancer deaths are estimated because the prevailing winds carry a large fraction of the effluent over the Atlantic Ocean. The individual risk of dying from respiratory cancer from the east central siting scenario is about 2×10^{-10} /yr and a lifetime probability of about 2×10^{-8} . Even though all of these estimates are very small, siting of the facilities can alter the calculated death rate by a factor of about 3.

6.1.3 Shortcomings of Coke Oven Data Model

Biological activity of coal-derived materials tends to be higher for the higher boiling materials in the temperature range between 450-1050°F (Pelroy and Wilson 1981). Lloyd (1971) noted the apparent relationship between carbonization temperatures and increased lung cancer incidence. Recent data from several laboratories indicate that distillates derived from the SRC-I, H-coal, and Exxon Donor Solvent process show little mutagenicity, cell transforming activity, or carcinogenicity when boiling points are below 600°F. Coke oven emission data are not presently reported as a function of source material boiling point as are the coal liquefaction releases. The boiling point distribution of coke oven emissions, from which our dose-response function was calculated, is not known, and therefore the above estimated cancer deaths may be conservatively high and may be reduced by considering only the NMHC, which boil above 600°F.

A finer definition of potential risks from coal liquefaction emissions requires an improved data base. The data base should include chemical characterization and quantitative measurements of any products, by-products or emissions used as surrogates.

6.2 MATRIX APPROACH

The matrix approach may improve the assessment of risks to human health from a coal liquefaction industry. The most reliable data on health risks is from epidemiological studies of workers within the industry. For example, health effects produced by coke oven emissions have been, to some extent, quantitated and correlated with exposure levels. The lack of a mature coal liquefaction industry precludes obtaining similar data. Therefore, a method is needed to link epidemiologic data such as is available for coke oven workers, roofing tar workers, etc., to data available for coal liquefaction processes. Since extensive biological and chemical characterization data are available for coal liquefaction materials, we propose construction of a multi-dimensional matrix, which includes chemical, biological, and epidemiologic data. The biological and chemical data would provide the link with epidemiologic data available for other coal-derived materials and allow estimation of health risks from exposure to coal liquefaction materials. Although we derived the matrix concept independently, it is essentially the same, except for the consideration of chemical properties, as that proposed by Cuddihy et al. (1980) for diesel exhaust assessment.

The proposed matrix concept is a subjective statistical approach. A purely objective analysis would require an unmanageable and unavailable data base. The matrix will be used to statistically test the intuitive hypotheses derived from biological events observed in the laboratory which may link chemical and epidemiological data.

We believe that two classes of materials may be good candidates for initial evaluation in this scheme, the neutral PAHs and the nitrogen-containing PAHs. Chemical analyses have shown that both classes increase monotonically with boiling point to temperatures in excess of 1000°F. Extensive biological studies have shown that microbial mutagenesis, mammalian cell transformation, and skin carcinogenicity also increase with increasing boiling point, with large increases in activities found above 700°F. These studies suggest that major emphasis can be placed on constituents having relatively large condensed ring systems (4 rings or greater).

Data comparing carbon-to-hydrogen ratios of coal liquefaction and coking aerosols could be examined to better understand the applicability of existing epidemiological data. Dose-response functions for NMHC based upon concentrations of nitrogen-containing polyaromatic compounds in higher boiling coal liquid fractions is also needed to fill data gaps in the matrix. The large body of data on coke oven and coal tar products and asphalt workers would be more useful if this information were available (NIOSH 1973; NIOSH 1977a,b).

7.0 UNCERTAINTY IN THE ASSESSMENT

There are three areas of uncertainty in most studies of this nature:

1. available models and numerical values
2. identified areas in models that can not be quantified at present*
3. factors in the assessment that have not been identified yet.

At this stage in the zero-order assessment, we have attempted to work with the first area of uncertainty. The first area will be further refined, and the second and third areas will be explored in the next iteration of this report.

Health effects estimates are based on the specification of a dose-response function and the computation of population exposure estimates due to NMHC (>600°F) releases to the atmosphere. A linear, nonthreshold dose-response function D is assumed. Population exposure estimates are obtained from the Pacific Northwest Laboratory long-range transport model for respirable particulates and the transport matrix derived from it (Eadie and Davis 1979). A general discussion on transport matrix concepts has been reported by DOE (1981b). Using the notation from the latter, the national population exposure (NPE) is defined by

$$NPE = \sum_{i=1}^n P_i C_i = \sum_{i=1}^n P_i \sum_{j=1}^n T_{ij} E_j$$

where

P_i = population for receptor region i

C_i = predicted concentration of NMHC for receptor region i

E_j = emission rate of NMHC precursor(s) from emitter region j

T_{ij} = transport potential from emitter region j to receptor region i .

* A good example of this category is: How will the airborne aerosol of NMHC change chemically and physically as a function of transport distance and time?

An estimate of potential human health effect is given by

$$H = D(NPE)$$

The uncertainty in the health effect estimate is assessed by considering the uncertainty in the individual components and their assumed relationship. The key areas of uncertainty are

- . source emission rates
- . transport matrix coefficients
- . population estimates
- . dose-response function.

In the current study the relationship among these components will be assumed correct.

NMHC releases to the atmosphere with boiling point fractions above 600 F are estimated as 0.6 g/sec for fugitive emissions. Weber and Craun (1982) critically evaluated the uncertainty in the estimation of fugitive volatile organic compound emissions. They arrived at an uncertainty of a factor of 3. They also stated a possible bias (discrepancy between the value expected and actual "true" value) of one order of magnitude due to the boiling point assumption. We assume that the uncertainty in the routine emissions are also a factor of 3. For each emitting region, the emission rate and the uncertainty is the same. If E is the common emission rate, then

$$NPE = E \left(\sum_{i=1}^n \sum_j P_i T_{ij} \right) = E (P)$$

where P is the population exposure potential for the coal liquefaction emitting regions.

The uncertainty in population exposure potential combines the uncertainty in population estimates for AQCR and the uncertainty in the transport matrix coefficients. It is assumed in this assessment that there is no uncertainty in the population projections. In computing population exposure potential, only the total U.S. population and the relative size of AQCR populations are important. Although uncertainty in these quantities exist, they are small compared to other sources. The population can also be regarded as a reference population.

The uncertainty in population exposure potential P is due to the transport matrix coefficient uncertainty. No validation of the matrix methodology has been completed for PNL's long-range trajectory model for respirable particulates (DOE 1981b). Limitations in emission data and observed concentrations severely restricts such a validation. No firm basis for an uncertainty estimate exists. Based on a general assessment of the capability of long-range transport models, an uncertainty ranging from a factor of 2 to 5 is assumed with a factor of 3 used as typical.

The uncertainty in the dose-response function arises from the uncertainty in the integrated dose received by the coke oven workers and from the translation of those exposure data to NMHC exposures from coal liquefaction. A lower limit estimate of uncertainty for the dose-response function is a factor of 2. No explicit calculation of an uncertainty was possible without examination of the data in detail. It is recognized that additional uncertainty is introduced when estimates based on small populations are extrapolated to much larger populations; i.e., U.S. population.

Uncertainty is not a universally well defined concept. Typically, uncertainty in an estimate includes two components: bias and variability. Both components are difficult, if not impossible, to quantify in assessment methodology. Estimates for the assessment are based on a limited amount of data. Because of the limited data, variation due to random fluctuations causes the estimated value to differ from the value expected if unlimited data were available. This variability is measured as the square of the standard deviation. Bias is a measure of the discrepancy between the value expected and the actual "true" value. Precision and accuracy, as commonly used in physical science literature, are similar concepts. An example of

variability is the uncertainty in the statistical estimate of the dose-response value for coke oven workers. A possible source of bias is translating the coke oven dose-response to coal liquefaction NMHC exposure. An attempt to include both components in the uncertainty calculations has been made.

A simplified uncertainty calculation can be based on the equation

$$H = D(NPE) = D(E)P$$

where D is the dose-response function and H is the estimated health impact. If U_x is the uncertainty for factor x, then the uncertainty in health impact is approximated by

$$U_H = \sqrt{U_D^2 + U_E^2 + U_P^2}$$

Given the uncertainties previously described, the uncertainty in health impact is approximately a factor of 4.7. This assumes the uncertainties are additive for each factor and the error distributions are approximately symmetric or Gaussian.

An alternative formulation is to assume the uncertainties for each factor are multiplicative and their distributions are approximated by a log-normal distribution. Under these assumptions, the uncertainties in the health impact is estimated as

$$U_{\ln H} = \sqrt{U_{\ln D}^2 + U_{\ln E}^2 + U_{\ln P}^2}$$

$$\text{and } U_H = e^{U_{\ln H}}$$

Given the uncertainties previously described, the resulting uncertainty is approximately a factor of 5.5.

Therefore, we have chosen a factor of 5 to express the total minimum uncertainty in the present estimate of the excess human lung cancer deaths that may result from the inhalation of released high-boiling nonmethane hydrocarbons during the synfuel production scenario presented here.

8.0 CRITICAL ASSUMPTIONS

Several assumptions were made during this assessment that could have enormous impact upon estimates of health effects and the uncertainty about the estimates. Many of these assumptions will be further investigated in the second and third iterations of this assessment. In addition, the scope of the assessment will be expanded. Examples of critical assumptions include:

1. NMHC - Only one class of emissions were evaluated from direct coal liquefaction. Others that would be included in later iterations would be criteria air pollutants, heavy metals, and a variety of other contaminants from wastewater discharges.

2. The Inhalation Pathway was considered for this assessment. In later iterations both aquatic and terrestrial exposure pathways will also be investigated.

3. There are tumor promoters in fractions of NMHC that boil below 600°F. Only the collection of more research data on these promoters can impact the assumption that we should primarily be covered with the NMHC fractions that boil above 600°F.

4. It is assumed that coke oven emissions and coal liquefaction emissions are chemically and physically similar.

5. Exposure estimates derived from the coke oven studies can be used to approximate exposures associated with coal liquefaction.

6. Risks of lung cancer in coke oven workers have been adequately determined, especially the dose-response relationship.

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APPENDIX A
NEAR-FIELD DISPERSION MODEL

A sector averaged Gaussian plume model was used to compute average annual pollutant air concentrations within a hypothetical facility site. The model is based directly on algorithms documented by Busse and Zimmerman (1973) as applicable multiple releases in a rural region.

The average concentration $\bar{C}_n$ resulting from a single source n is given by

$$\bar{C}_n = \frac{16}{2\pi} \sum_{\ell=1}^6 \sum_{m=1}^6 \frac{\phi(k_n, \ell, m) G_n S(\rho_n, z, U_\ell, P_m)}{\rho_n}, \text{ g/m}^3 \quad (1)$$

where

- k_n = wind sector appropriate to the n^{th} point source
- G_n = emission rate of the n^{th} point source, g/sec
- ρ_n = distance from the receptor to the n^{th} point source, m
- ℓ = index identifying the wind speed class
- m = index identifying the class of the Pasquill stability category
- $\phi(k_n, \ell, m)$ = joint frequency function
- $S(\rho_n, z, U_\ell, P_m)$ = dispersion function defined in Equation 3, sec/m³
- z = height of receptor above ground level, m
- U_ℓ = representative wind speed, m/sec
- P_m = Pasquill stability category

The average concentration $\bar{C}_t$ resulting from multiple sources s is given by:

$$\bar{C}_t = \sum_{n=1}^s \bar{C}_n, \text{ g/m}^3 \quad (2)$$

The receptor is assumed to be at ground level, that is $z = 0$, making the dispersion function

$$S(\rho_n, 0, U_\ell, P_m) = \frac{2}{\sqrt{2\pi} U_\ell \sigma_z(\rho_n)} \exp \left[-\frac{1}{2} \left(\frac{h}{\sigma_z(\rho_n)} \right)^2 \right] \exp \left(\frac{-0.693 \rho_n}{U_\ell T_{1/2}} \right) \quad (3)$$

New terms in Equation 3 are defined as

$\sigma_z(\rho_n)$ = vertical dispersion function, i.e., the normalized standard deviation of the NMHC concentration in the vertical plane, m

h = effective stack height of source, m

$T_{1/2}$ = half time, sec

The values of vertical dispersion parameter in the six Pasquill stability categories as a function of downwind distance are taken directly from Busse and Zimmerman (1973). These values represent passive atmospheric dispersion of a point source release.

Initial dispersion will be controlled by wake effects of the building from which releases occur. Building wake effects are accounted for by computing an adjusted vertical dispersion parameter, σ'_z . A formulation given by Slade (1968) was used,

$$\sigma'_z = \left[\sigma_z^2 + \left(\frac{cA}{\pi} \right)^2 \right]^{1/2} \quad (4)$$

where A = cross sectional area of building normal to wind, m^2

c = empirical constant.

The buildings are assumed to be six meters high for purposes of computing an input area. An average area is used for all computations. The reported values of c vary between 0.5 and 2.0; 0.5 was used here.

The exponential term in Equation 3 with the $T_{1/2}$ value represents the chemical half time of the pollutant. This exponential term was assumed to be unity--that is no chemical changes are assumed. Although the validity of this assumption depends on the composition of the releases, assuming no changes provides an upper limit estimate of concentration.

Concentration patterns are computed using the above equations for five ground-level releases of 0.24 g/s each at each of the five release points shown on the site map (Figure 5.1).

As generic meteorological data, a one-year joint wind speed, direction and stability summary is selected from near Oak Ridge, Tennessee. Stability is derived from vertical temperature gradients. This is used to show typical results only. These meteorological data are not intended to be specific for any proposed site.

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APPENDIX B
PNL LONG-RANGE TRANSPORT MODEL

The PNL Long-Range Transport (LTR) model is a regional-scale transport, transformation and removal model developed by Wendell et al. (1976) and adapted by Eadie and Davis (1979) for generation of air quality control region (AQCR) interregional transport matrices. Sensitivity and verification studies with the LRT model have been conducted by Powell et al. (1979) and D. J. McNaughton (1980) for sulfur dioxide and sulfate air concentrations and depositions in the northeastern United States.

The PNL advection grid (see Figure B.1) upon which layer-averaged winds are mapped every 12 hr is a subset of the National Meteorological Center (NMC) grid and spans the United States and adjacent areas. Trajectories are simulated for plume elements released hourly from an emission source location. The unit emission rate at the source position determines the initial fine particle mass of each plume element. Subsequent horizontal transport of these plume elements is in hourly steps using the layer-averaged winds at each advection-grid intersection point. An objective analysis scheme developed for mesoscale purposes (Wendell 1972) interpolates wind data in space and time to provide the hourly winds at each particle position. The current transport scheme has no vertical component. It is assumed that the concentrations of fine particulates are averaged over a time period in which the effects of vertical atmospheric processes can be adequately expressed by the parameterized vertical component of diffusion and by the mixing depth constraints. It is also assumed that the effects of vertical transport on horizontal transport can be neglected over the long assessment time period.

The removal of fine particles from the atmosphere by dry and wet deposition are calculated by a set of ordinary linear differential equations that are solved for each plume element. These equations assume that the dry-removal rate is obtained by multiplying the deposition velocity by a vertical distribution factor and the wet-removal rate is a function of the local precipitation rate mapped on the sampling grid.

FIGURE B.1. PNL Advection Grid and Grid-Point Source Locations

The AQCR to AQCR interregional transport matrices are generated by first running the LRT model, using a single month of meteorology, for 86 "base" unit sources represented as dots in Figure B.1. The sources are assumed to be 200 meters high which includes plume rise. This source height was chosen as an aggregated representative height for all source categories. The results of the model run are monthly averaged air concentration fields on the 32 kilometer square grid system covering the United States. Each concentration field represents the impact from each of the 86 base unit sources.

Next a " $1/R^2$ " interpolation scheme is used to produce concentration fields from the base concentration fields for 238 unit sources located at the area centroid of each of the AQCRs in the contiguous United States as shown in Figure B.2. The distance between the base unit source, i , and an AQCR unit source is represented by R_i . Briefly, the method involves weighting the concentration fields of the four closest base unit sources to the AQCR unit source by a function w , translating each base unit source concentration

FIGURE B.2. United States Environmental Protection Agency
Air Quality Control Region Centroids

field by the corresponding distance R_i , and then summing to arrive at an AQCR unit source concentration field. The weighting function, w , used for this purpose is:

$$\frac{1/R_i^2}{\sum_{i=1}^4 (1/R_i^2)}$$

This interpolation method is very appealing because of the savings in computing time by not having to run the LRT model for all 238 sources.

The final step in the generation of the matrices is the averaging of the respective portions of the "emitter" AQCR concentration field residing in the other 237 "receptor" AQCRs. A population weighting method is used to accomplish this averaging. Basically, the procedure involves multiplying the fine particulate air concentration for each grid box in a receptor AQCR by a population-weighting factor for that grid box, and summing the resulting products for all grid boxes within the receptor AQCR. This procedure is repeated for every combination of emitter and receptor AQCRs. The population-weighting factor is equal to the population in the grid box residing within an AQCR divided by the total population residing within that AQCR. The Brookhaven National Laboratory (BNL) population projections, based on 1970 U.S. census data, for the year 1985 are used to calculate the population weighting factors.

AQCR to AQCR interregional transport matrices of population-weighted, monthly averaged fine particle air concentrations have been generated for four months of meteorology, January, April, July and October 1974. In addition, the matrices for the four months were averaged to produce a transfer matrix roughly approximating annual average impacts. Table B.1 gives a summary of LRT model parameters used for generation of the matrices.

TABLE B.1. Long-Range Transport Model Parameters for Generation of Fine Particulate AQCR-to-AQCR Matrices

Long-Range Transport Model Parameters	
Time periods for meteorological data	1-31 January 1974 1-30 April 1974 1-31 July 1974 1-31 October 1974
Advection grid spacing (35 N latitude)	321 km
Grid spacing for sampling of results and for precipitation data (35 N latitude)	32 km
Source emission rate	1.0 kiloton/yr
	Advection grid intersections for interpolation to centroids of AQCR
Effective source stack height	200 m
Maximum daytime mixing height	1500 m
Minimum daytime mixing height	200 m
Maximum nighttime stable layer height	400 m
Minimum nighttime stable layer height	100 m
Stability	Varied through the diurnal cycle
Dry deposition velocity	0.23 cm/sec
Wet removal	.38 p.73/hr, where P = rainfall rate in mm/hr
Puff release rate from source, advec- tion time step, and sampling rate of puffs for results	1 per hr
Maximum number of hours a puff trajec- tory will be continued if it stays on grid	200 hr
Averaging period for air concentra- tion fields of fine particulates	1 mo
Units of air concentrations of fine particulates	g/m ³ g/m ³

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