PROJECT SUMMARY:

ENVIRONMENTAL ASPECTS OF SYNFUEL UTILIZATION

December 1980

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M. Ghassemi and R. Iyer

TRW

ENVIRONMENTAL ENGINEERING DIVISION
Redondo Beach, CA 90278

EPA Contract No. 68-02-3174
Work Assignment No. 018
EPA Program Element No. CCZN1A

Project Officer: J. McSorley

Industrial Environmental Research Laboratory
Office of Environmental Engineering and Technology
Research Triangle Park, N.C. 27711

Prepared for:

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This study reviews the environmental concerns relating to the distribution, handling, and end use of synfuel products likely to enter the marketplace by the year 2000, and assigns priority rankings to these products based on environmental concerns to aid EPA in focusing its regulatory and research activities. Major products and by-products from oil shale, coal liquefaction, and coal gasification technologies are considered.

Based on current developmental activities, three likely scenarios for shale and coal-based synfuel plant buildup are projected. The type and quantity of synfuel products and by-products likely to enter the market are identified and their regional market penetration is estimated. The environmental analysis consists of a review of the available data on the physical, chemical, and health effects characteristics of synfuel products and environmental significance of the characteristics; an analysis of the potential environmental impacts and regional implications associated with the production and use scenarios considered; and a ranking of the products from the standpoint of environmental concerns and mitigation requirements.

The results indicate that: (a) significant quantities of synfuel products are expected to enter the marketplace during the next 20 years; (b) large-scale transportation, distribution, and end use of certain synfuel products can present significant threats to the environment and the public health; (c) based on gross characteristics, synfuel products appear to be similar to petroleum products, but detailed characterization data are not available with which to judge their relative safety; and (d) synfuel test and evaluation programs currently under way or planned provide excellent opportunities for collecting some of the required environmental data.

This is a summary of the complete project report, which can be purchased from the National Technical Information Service.

INTRODUCTION

To date, most synfuel-related environmental assessment programs have focused on the technologies for synfuel production and on emissions from production facilities. The present study constitutes the first major effort by EPA to examine environmental concerns that would be associated with the projected widespread utilization of synfuel products. A related EPA program, currently under way, extends the effort to an analysis of the trade-offs of various product slates for minimizing end use environmental impacts.

The present study consists of: (1) a projection of synfuel production and product utilization over the next twenty years, and (2) a ranking of products from the standpoint of environmental concerns. The data base used consists of information obtained from major process developers, potential product users, and published literature.

CANDIDATE TECHNOLOGIES AND PRODUCTS

Synfuel technologies likely to be used in commercial plants over the next 20 years are oil shale, coal gasification (low-/medium-Btu and SNG) and coal liquefaction (direct and indirect). Brief descriptions of these technologies and their development status are presented in Table 1. Major products and by-products of these technologies and their anticipated general uses are indicated in Figure 1; their specific likely end uses are listed in Table 2.

SYNFUEL INDUSTRY BUILDUP SCENARIOS

The development of a synfuel industry in the U.S. within the next 20 years will be influenced by a large number of factors, the most important of which are:

- Availability of capital for financing the massive construction costs
- Willingness of process developers, the private investment sector and government to accept the technological risks involved in the construction of the "first-of-a-kind" integrated coal and shale facilities
- U. S. Government energy policies and prices of domestic and imported natural gas and oil
- Availability of skilled manpower, raw material, and equipment for plant construction and operation
- Timely development of the supporting infrastructure necessary for energy product manufacture, distribution, and use
- Environmental regulatory requirements, and the time and effort required to acquire technical data to support permit applications and obtain approval
- Effort and time required to attain full commercial status for technologies/processes currently under development.

TABLE 1. CANDIDATE SYNFUEL TECHNOLOGIES AND THEIR STATUS OF DEVELOPMENT

Technology	DESCRIPTION	DEVELOPMENT STATUS
Oil Shale	• Heating oil shale to about 480°C to extract shale oil • Heating accomplished via surface retorting, in situ retorting or modified in situ retorting • Crude shale oil can be upgraded to produce syncrude for use as refinery feedstocks or boiler fuel	• Closest to commercialization of all synfuel technologies for production of large volumes of liquid fuels • Surface retorting more advanced than in-situ retorting • All technologies demonstrated at pilot scale or larger • Several production facilities planned for operation in 1980's
Direct Coal Liquefaction	• Coal, hydrogen and a coal-derived liquid mixed at high temperature and pressure to produce additional coal-derived oil, which is separated and refined to liquid fuels • Three major processes under development SRC II, H-coal and Exxon Donor Solvent (EDS) Processes differ in the way hydrogen is made to react with coal	• SRC II Pilot plant under operation, 6700-ton/day of coal demonstration unit under design and scheduled for operation in 1984-85 • H-Coal 600-ton/day of coal pilot plant under construction, testing to begin soon • EDS 250-ton/day of coal pilot unit under construction, testing to begin soon
Indirect Coal Liquefaction	• Coal reacted with oxygen and steam in a gasifier to produce a synthesis gas, after removal of CO_2 and other impurities, CO and H_2 in the gas reacted catalytically to produce several products ranging from lightweight gases to heavy fuel oil (Fischer-Tropsch process) or to methanol which is then converted to gasoline (Mobil-M process)	• Fischer-Tropsch 8000-ton/day of coal plant (SASOL I) producing over 10,000 bbl/day of liquids in commercial operation since 1956 in South Africa, a 40,000-ton/day of coal unit (SASOL-II) will begin operation soon • Mobil-M Commercial plant to produce 12,500 bbl/day of gasoline from reformed natural gas planned for New Zealand in 1984-85
Coal Gasification	• Reacting coal, steam and air/oxygen to produce low-Btu (80-150 Btu/scf) or medium-Btu(300-500 Btu/scf) gas, medium-Btu gas purified and upgraded to SNG (∿1000 Btu/scf) • Gasifiers differ in design and operation, depending on type of coal used and products desired	• Low-Btu gas Extensive commercial experience in U S with gasifiers operating near atmospheric pressure, applications are small-scale operations producing gas for captive use in industrial and process heating • Medium-Btu gas extensive commercial experience exists for Lurgi fixed-bed process, several projects using the Texaco process for captive applications (chemical feedstocks and on-site power generation) in planning and design stages • High-Btu gas plans for SNG production using Lurgi technology announced by pipeline and gas utility companies

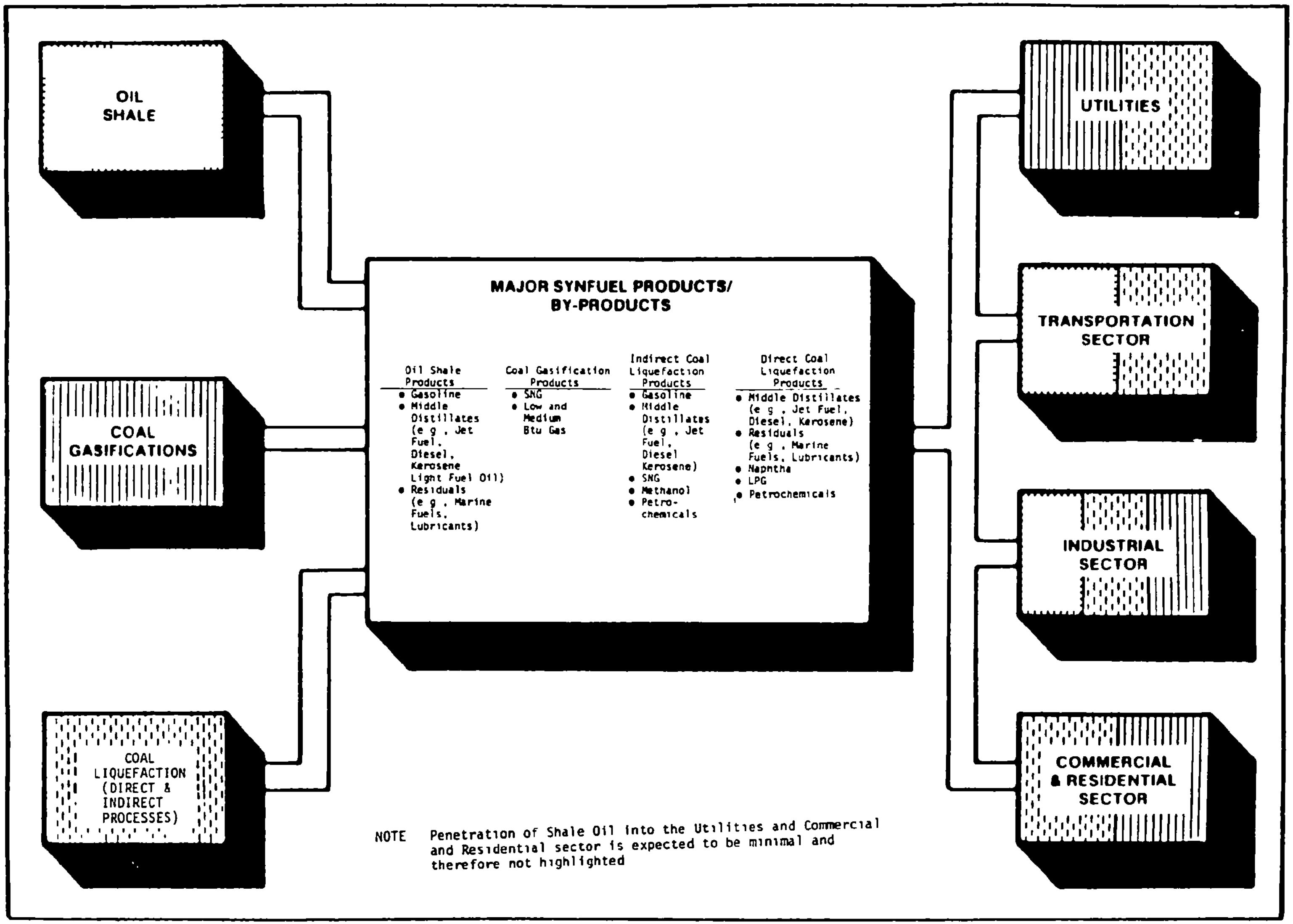

FIGURE 1. SYNFUEL UTILIZATION DURING 1985-2000

Table 2. MAJOR END USE APPLICATIONS OF SYNFUEL PRODUCTS

Major Synfuel Products	Likely Major End Use Applications
High- and medium-Btu gas	Food, textile, pulp and paper, chemicals, iron and steel industries; residential/commercial heating
Low-Btu gas LPG	Small boilers, kilns, pelletizing glass, electronics, chemical industries; domestic cooking and heating; automotive
Gasoline	Transportation
Naphtha	Petrochemical industry; solvents; varnish; turpentines
Middle distillates (kerosene, diesel, light fuel oil)	Transportation, gas turbines, residential and commercial heating
Residues	Industrial, utility and marine fuel; metallurgical oils; roof coatings; wood preservatives, lubricants

Based on different assumed levels of impacts exerted by these factors, three scenarios or forecasts for synfuel industry buildup to the year 2000 were developed. These scenarios are:

- National goal scenario driven by federal incentives (Scenario I; medium buildup rate)
- Nominal production scenario (Scenario II; low buildup rate)
- Accelerated production scenario representing an upper bound for industry buildup (Scenario III; high buildup rate).

The scenarios, shown in Figure 2, project the total quantities of shale oil, low-/medium-Btu gas, high-Btu gas and liquids from coal that would be expected to enter the market under the assumed sets of conditions. Based on discussions with major synfuel suppliers and users and industry and government planners, Scenario II was selected as the more realistic of the three scenarios and was used for analysis of regional impacts and environmental issues. This scenario is consistent with the general consensus among technical experts and potential major suppliers that shale oil is more nearly cost competitive and closer to commercialization than

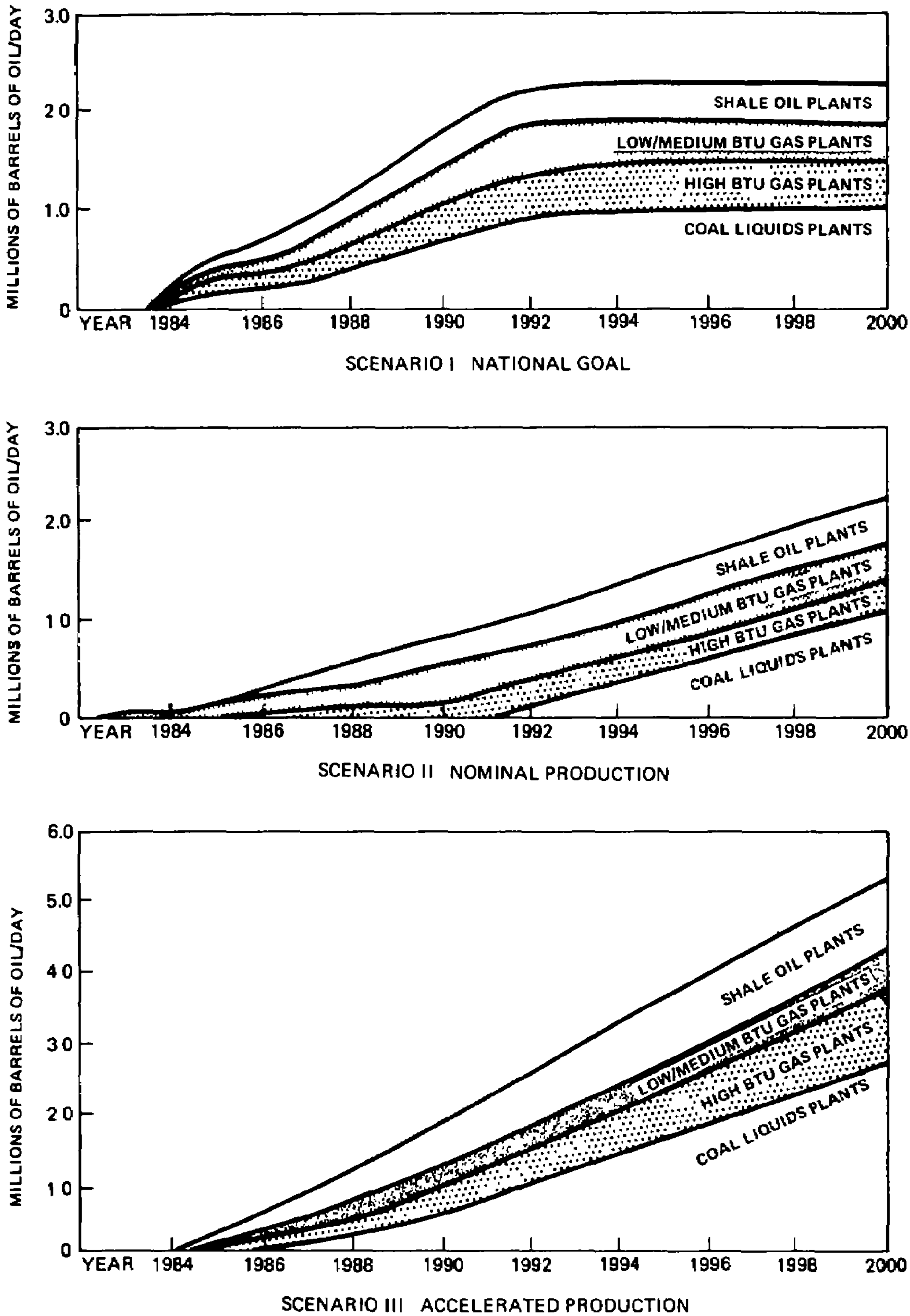

FIGURE 2. FORECASTS FOR SYNFUEL INDUSTRY BUILD-UP

high-Btu gasification or coal liquefaction, and that commercial coal liquefaction facilities will not probably come on-line before the early 1990's. Synfuel industry buildup and product utilization patterns are analyzed for three time frames: 1980-1987, 1988-1992, and 1993-2000. Table 3 presents the product-by-product estimates of synfuel utilization in the U.S. For comparison, the estimated quantities are also expressed as percentages of the total amount of products (synfuel and non-synfuel) used.

It should be noted that, even though on a national scale, the projected synfuel utilization would account for small fractions of the total product usage, in some regions a very high fraction of the currently used products are expected to be replaced by synfuel products. As noted in Table 4, by the year 2000 it is expected that 36 percent of all refinery feed and 48 percent of all middle distillate used in EPA Region VIII would originate from shale oil.

TABLE 4. PROJECTED UTILIZATION OF SHALE OIL PRODUCTS IN EPA REGION VIII (REGION OF MAXIMUM PRODUCT USE) AS PERCENTAGES OF TOTAL PRODUCT QUANTITIES USED

PRODUCT	1980-1987	1988-1992 & 1993-2000
Crude (fuel)	1.3	-
Refinery Feed	13.3	35.6
Middle Distillate	37.6	48.3
Gasoline	4.8	2.3
Residuals	15.6	6.6

SYNFUEL PRODUCT UTILIZATION AND EPA REGIONS OF MAXIMUM IMPACT

EPA regions where synfuel products would most likely be utilized are identified in Figure 3. Table 5 summarizes the projections of synfuel product utilization patterns in the EPA regions impacted. As noted in the table, except for oil shale in the 1988-1992 and 1993-2000 time frames and for direct coal liquefaction in the 1993-2000 time period, the transportation, distribution, and use of products are expected to be confined to the regions where each synfuel is produced. Consequently, environmental impacts associated with product utilization are expected to be confined primarily to the production regions, except for impacts associated with the natural transporation of pollutants across regional boundaries (for example, transportation of air pollutants emitted from combustion sources). The projections indicate that up to the year 2000

TABLE 3. ESTIMATED QUANTITY OF SYNFUEL PRODUCTS USED IN THE U.S. UNDER SCENARIO II

Product	1980-1987		1988-1992		1993-2000	
	Amount (MMBPD)	% of total in U. S.	Amount (MMBPD)	% of total in U. S.	Amount (MMBPD)	% of total in U. S.
Crude shale oil (fuel)	0.0008	0.05	0	0	0	0
Shale oil refinery feed	0.07	0.45	0.41	0.24	0.43	2.4
Shale jet fuel	0.015	1.2	0.09	6.5	0.09	6.8
Shale diesel fuel	0.042	1.2	0.23	6.5	0.23	6.8
Shale residuals	0.007	0.2	0.04	1.3	0.04	1.3
Shale gasoline	0.13	0.2	0.07	0.9	0	0
Medium-Btu gas (coal)	0.09	0.9	0.27	2.8	0.45	4.7
SNG (coal)	0.042	0.4	0.17	1.8	0.25	2.6
Gasifier tars, oils	0.004	0.04	0.01	0.1	0.01	0.1
Gasifier phenol	0.004	0.04	0.01	0.1	0.02	0.2
F-T LPG	0	0	0	0	0	0
F-T medium Btu gas	0	0	0.01	0.06	0.01	0.1
F-T SNG	0	0	0.03	0.33	0.07	0.7
F-T heavy fuel oil	0	0	0.001	0.02	0.001	0.03
F-T gasoline	0	0	0.02	0.2	0.03	0.4
Mobil-gasoline	0	0	0.05	0.66	0.1	1.3
F-T diesel fuel	0	0	0.002	0.04	0.01	0.1
Fuel methanol	0	0	0.14	1.8	0.23	3.0
SRC II fuel oil	0	0	0.03	0.3	0.09	1.3
SRC II naphtha	0	0	0.02	0.2	0.05	0.8
SRC II LPG	0	0	0.006	0.4	0.02	1.6
EDS fuel oil	0	0	0	0	0.06	1.0
EDS naphtha	0	0	0	0	0.03	0.6
EDS LPG	0	0	0	0	0.01	0.9
H-coal fuel oil	0	0	0	0	0.06	0.4
H-coal naphtha	0	0	0	0	0.03	0.2
H-coal LPG	0	0	0	0	0.01	0.1

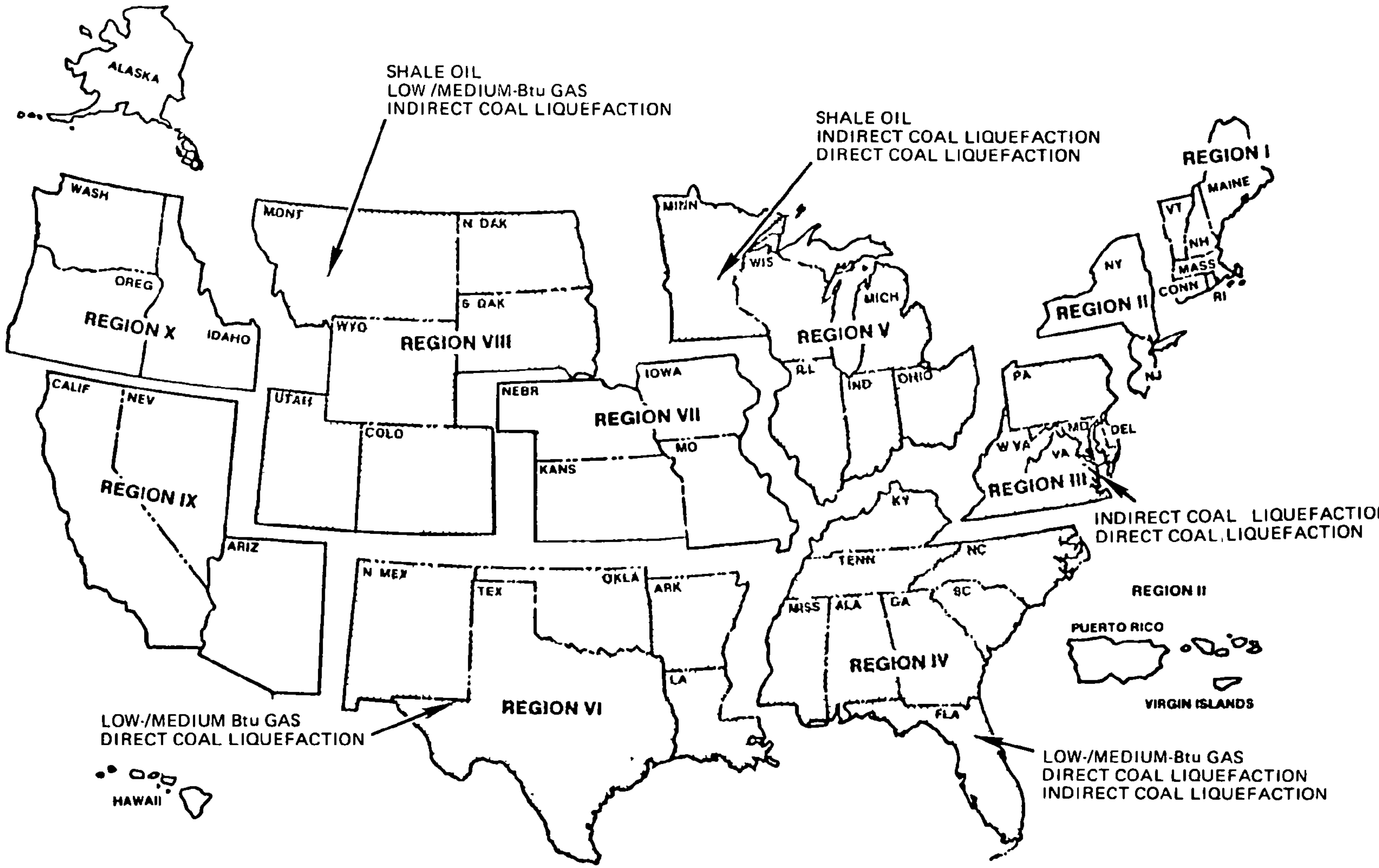

Figure 3. EPA Regions of Synfuel Products Utilization (1990's)

TABLE 5. ESTIMATED UTILIZATION PATTERNS FOR SYNFUEL PRODUCTS IN EPA REGIONS IMPACTED*

Synfuel	Time Frame	Production	Refining	Utilization/Products	
Shale Oil	1980-1987	VIII†	VIII	VIII	mid distillate (57), gasoline (13), residuals (7)
	1988-1992/ 1993-2000	VIII(410)	VIII(210)	VIII	mid distillate (155), gasoline (36), residuals (19)
			V (200)	V	residuals (18)
				V & VII.	mid distillate (148), gasoline (34)
Low-/medium-Btu Coal gas	1980-1987‡	IV(30)	-	IV.	gas (30)§
		VI(30)	-	VI	gas (30), tars/oils (0 98-1 9), phenols (0 15-0.30), naphtha (0.25-0 72)
		VIII(30)	-	VIII	gas (30), tars/oils (0.98-1 9), phenols (0.15-0 30), naphtha (0.25-0.72)
Indirect Coal Liquefaction Products	1988-1993	VIII(100)	VIII(100)	VIII	gasoline (64 5), mid distillates (2.5), residuals (0 7), SNG (32 6), LPG (0.1), tars/oils and phenols
	1993-2000	VIII(200)	VIII(200)	VIII.	gasoline (129), SNG (65.2), diesel fuel (5 0), residuals (1.4), LPG (0.2)
		IV(150)	IV(150)	IV	gasoline (150)
		III(300)	III(300)	III.	gasoline (300)
Direct Coal Liquefaction Products	1988-1992	V(50)	V(50)	V	naphtha (15.4), mid distillate (18.7), residuals (10), LPG (5.9)
	1993-2000	III(50)	III(50)	III	naphtha (15 4), mid distillate (18.7), residuals (10), LPG (4 5)
		IV (100)	IV (100)	VI	LPG (10.6)
		V (200)	V (200)	IV	mid distillate (37 4), naphtha (30.8), residuals (20.0), LPG (9.0)
				V	naphtha (61 6), mid distillate (74.8), residuals (40.0), LPG (20 2)

* numbers shown in paranthesis are product quantities in 10^3 BPC oil equivalents

† See Figure 3 for states covered by each EPA region

‡ Production and utilization patterns for 1988-1992 and 1993-2000 are the same as shown

§ Use of Texaco process, which does not generate tars, oils and phenols, is anticipated under Scenario II, the environmental impacts of synfuel product utilization would be expected to be largely limited to EPA Regions V and VIII for oil shale; to EPA Regions IV, VI, and VIII for medium-Btu gas; to EPA Regions III, IV, and VIII for indirect coal liquefaction products, and to EPA Regions III, IV, and V for direct liquefaction products.

ENVIRONMENTALLY SIGNIFICANT CHARACTERISTICS OF SYNFUEL PRODUCTS

The environmental and health effects data currently available on synfuel products are very limited and pertain mainly to certain primary products (for example, crude shale oil or coal liquefaction syncrudes). Very little data are available on many of the secondary synfuel products (for example, methanol and gasoline derived from coal) or on emissions associated with end uses. Several combustion tests conducted with synfuel products (primarily shale oil fuels) have been aimed primarily at the evaluation of handling and performance characteristics. In general, the product/emissions characterization has been in terms of gross properties (for example, ultimate analysis, composition by chemical class, and emissions of smoke and particulates during combustion), which by themselves do not provide an adequate basis for assessing environmental significance. The current product characterization data base is a collection of results of sampling and analysis and performance testing that have been conducted by different investigators using samples/batches of products obtained from pilot plants operated under varying conditions. Accordingly, significant inconsistencies exist in the reported results, which further hamper assessment of the environmental safety of synfuel product utilization. This assessment is also hindered by a lack of data on analogous petroleum and natural gas products that the synfuel products will replace and that, because of their large-scale and widespread utilization, have generally come to be viewed by the public as environmentally innocuous. To illustrate the type of data available on synfuel products, the reported data on the physical and chemical characteristics of direct coal liquefaction products and the combustion and health effects characteristics of SRC II fuel oils are summarized in Tables 6, 7, and 8, respectively.

Table 9 identifies the differences in chemical, combustion, and health effects characteristics of synfuel products and their petroleum analogs, based on the reported characterization data. As noted in the table, for the majority of products for which data are reported, these differences primarily relate to the higher content of aromatics and fuel bound nitrogen (FBN) and greater emissions of NOx during combustion. Although no test data for synfuel products are available, high concentrations of aromatics in fuels have been shown to enhance production of PNA's during combustion. No actual data have been reported on the specific substances that comprise the aromatic or FBN fractions in various synfuel products (or their petroleum counterparts). In the case of fuels, high aromaticity has been generally implicated in an increase in smoke production; the limited combustion data which are currently available, however, do not indicate that all aromatic synfuels have higher smoke levels. High FBN content can raise the level of NO_x emissions; the excess NO_x emissions of synfuels are believed to be correctable by combustion modifications. The nitrogen

TABLE 6. SUMMARY OF AVAILABLE DATA PERTAINING TO PHYSICAL AND CHEMICAL CHARACTERISTICS OF DIRECT COAL LIQUEFACTION PRODUCTS

- Syncrudes have lower viscosities and pour points than petroleum crudes. Kinematic viscosity at 100°F values of 2 2 and 1.1 to 1 6 cst for SRC II whole process oil and H-Coal syncrude, respectively (vs. 6.14 and 18 9 cst for an Arabian light and an Arabian heavy crude, respectively). A pour point value of -80°F for SRC II whole process oil (vs -30°F for the two Arabian crudes) The lower viscosities and pour points for syncrudes indicate better handling and transfer characteristics

- Syncrudes have a high nitrogen content (0 17 wt % for H-Coal using low sulfur coal to 0 85 wt % for SRC II whole process oil, vs. 0 1 wt % for crude oil). The nitrogen reduced to about 50 ppm by moderate hydrotreating and to less than 1 ppm by severe hydrotreating

- The sulfur content of raw syncrudes (0 04 to 0.49 wt.%) would classify them as low sulfur feed The sulfur content is reduced to about 20 ppm or less by hydrotreating

- SRC II whole process oil has an aromatic content of 55 volume % Included in that value is almost 9% phenols. The aromatic content is reduced to 49% by "intermediate severity" hydrotreating and to 4% by "severity hydrotreating"

- Naphtha from SRC II, H-Coal and EDS contain 16 2, 18.2, 18 6 and 25.3 vol % aromatics and 3 2, 3 1 and 7 4 vol % phenols, respectively Hydrotreatment appears to increase aromatic content and eliminate phenols. The hydrotreated naphtha from the three processes contain 19 to 21 vol % aromatics

- Direct liquefaction naphthas have low octane numbers (40 to 70) and hence are not suitable for direct use as gasoline Hydrotreating/platforming or hydrocracking/platforming produces gasoline stocks with octane numbers ranging from 91.5 to 99 8

- Gasoline or naphtha from direct liquefaction processes are less volatile than petroleum-derived leaded or unleaded gasoline The distillation end point for petroleum-derived gasoline is 340-345°F vs. 382-411°F and 365-459°F for liquefaction naphtha and gasoline, respectively

- Coal liquefaction naphtha can be processed to gasoline, having gross compositions (% aromatics, olefins, saturates, etc) similar to petroleum-derived gasoline.

- The oil distillates from EDS process are very low in nitrogen and sulfur (0 2-0.6 ppm and 2-139 ppm, respectively) Except for a lower gravity (2 5-27 9 vs. 30°) and higher flash point (136 vs 100°F), the distillates meet the specifications for No. 2 fuel oil.

- SRC II fuel oil (5 75 1 middle to heavy distillate ratio) is very similar to No. 6 fuel oil in characteristics, except for lower gravity (11° vs 25° API), heating value (17,081 vs 19,200 Btu/lb), pour point (-30°F vs. 95°F) and flash point (150 vs. 200°F) and higher nitrogen content (1.02 vs 0.23 wt %).

- Jet and diesel fuels obtained from H-coal and SRC II syncrudes meet the specifications for these products.

TABLE 7. COMBUSTION TEST RESULTS FOR SRC II FUEL OILS

Investigators	SRC II Fuels Tested*	Equipment/test	Results
Singh, et al (ASME Publication 80-GT-67, March, 1980)	MD, HD, MD/HD blend, 3 1 No 2/SRC II blend, 1 1 No 2/SRC II blend	Sub-scale gas-turbine like combustor	• All fuels burned well • no significant handling problem • max excess NO_x levels (with HD) 20 to 130 ppm above baseline • increase in smoke levels with decreasing hydrogen content & increasing aromaticity of fuels • decrease in % emissions of fuel-bound nitrogen (FBN) with increase in fuel FBN and outlet temperature
Bauserman, et al (Paper presented at Gas Turbine Conference, New Orleans, LA , March 10-13, 1980)	5·1 MD/HD	Full-scale combustor used in Westinghouse 30-to 90-MW engines, 187-h corrosion test using various alloys and SRC II solvent wash	• NO_x emission for blend containing 9 83% FBN 30 to 120 ppm higher than No. 2 distillates • decrease in smoke value with increase in exhaust temperature • corrosion/deposition problems similar to petroleum-derived products
Babcock and Wilcox Co (EPRI Report No FP-1028, June 1979)	5 75 1 MD/HD	Package boiler Ambient monitoring	• easy pumping/handling during test program (replaced hydrocarbon seals with teflon/viton seals as precaution) • no benzene/phenol emitted, based on ambient monitoring data • NO_x emissions for blend higher than for No.2 and No 5 • No tendency to smoke despite higher aromaticity • lower particulate emission in comparison with No 5 oil • ash composition for blend similar to that for No 5 oil except for Fe, Ca, Mg, Cr, Mn and Sn which were higher
KVB, Inc (EPRI Report No FP-1029, May 1979)	2 1 MD/HD	44-MW field boiler	• no major operation (burner optimization, boiler deposits,etc) problems in comparison with No 6 fuel oil • NO_x emissions about 70% higher than for No 6 fuel oil • lower particulate emissions compared to No 6 fuel oil, emissions less than proposed NSS of 0 03 lb/M Btu • PNA emissions for both blend and No 6 less than 6 μ/M^3 ($6x10^{-6}$ lb/M Btu) • tendency for incomplete combustion comparable to No 6 fuel oil (CO levels below 50 ppm)

*SRC II fuels MD = middle distillate HD = heavy distillate

TABLE 8. SUMMARY OF HEALTH EFFECTS DATA FOR SRC II PRODUCTS AND (WHERE AVAILABLE) FOR PETROLEUM ANALOGS

Test	Naphtha	Light Fuel Oil	Heavy Distillates
Ames Mutagenicity	No mutagenic activity for SRC II (revertants/μg < 0 01) or petroleum naphtha	No measurable mutagenic activity (revertants/μg < 0 01), mutagenic activity demonstrated for certain petroleum distillates	Most mutagenic of the three SRC II products (a 40 ± 23 revertants/μg)
Cytotoxicity (on cultured mammalian cells)	180 μg/ml dose required to produce a 50% reduction in relative plating efficiency (RPE), no comparative data for petroleum analog (RPE_{50} for crude petroleum 190-350 μg/ml)	RPE_{50} 200 μg/ml (vs 250 μg/ml for Diesel oil No 2 and 0 3 μg/ml for cadmium chloride)	with an RPE_{50} of 30 μg/ml, most cytoxic of all synfuel products tested, very active in effecting cell transformation
Skin-painting	As with petroleum naphtha extreme low tumorigenic activity, tumor incidence 1/46 at 20 mg/application after 456 days (vs 44/46 at 0 005 mg/application for benzo(a)pyrene, a known carcinogen)	—	highly potent*, 12% and 100% tumor incidents after 456 days at 0 23 and 2 3 mg/application, respectively, 85% of tumors malignant
Acute and subchronic toxicity	Moderately toxic Acute gavage rat LD_{50} 2 3 g/Kg, Subchronic (5 days) gavage rat LD_{50} 0 96 g/Kg	More toxic than diesel oil (acute rat LD_{50}=3 75 g/Kg vs 11 8 g/Kg), sub acute gavage rat LD_{50}=1 48 g/Kg	LD_{50} about the same as for naphtha and light fuel oil
Maternal and fetal toxicity (rats)	No significant enhanced toxicity to embryo or the fetus (risk only slightly higher than for the mother)	Same as for naphtha	Same as for naphtha
Toxicity via skin absorption	Unlike petroleum naphtha, shows some acute effect at a high dose levels (1 6 g/Kg)	Unlike the petroleum products, can cause skin burns	—

*No comparable data available for petroleum analog, but industrial fuels oils have been shown to present considerable skin carcinogenicity hazard.

TABLE 9. REPORTED KNOWN DIFFERENCES IN CHEMICAL, COMBUSTION AND HEALTH EFFECTS CHARACTERISTICS OF SYNFUELS PRODUCTS AND THEIR PETROLEUM ANALOGS

Product	Chemical Characteristics	Combustion Characteristics	Health Effects Characteristics
Shale oil			
Crude	Higher aromatics, FBN, As,Hg, Mn	Higher emissions of NO_x, particulate and (possibly) certain trace elements	More mutagenic, tumorigenic, cytotoxic
Gasoline	Higher aromatics	Slightly higher NO_x and smoke emissions	—
Jet fuels	Higher aromatics	Slightly higher NO_x and smoke emissions	Eye/skin irritation, skin sensitization same as for petroleum fuel
DFM	Higher aromatics	Slightly higher NO_x and smoke emissions	Eye/skin irritation, skin sensitization same as for petroleum fuel
Residuals	Higher aromatics	—	—
Direct Liquefaction			
Syncrude (H-Coal, SRC II, EDS)	Higher aromatics and nitrogen	—	—
SRC II fuel oil	Higher aromatics and nitrogen	Higher NO_x emissions	Middle distillates non-mutagenic, cytotoxicity similar to but toxicity greater than No 2 diesel fuel, burns skin Heavy distillate Considerable skin carcinogenicity, cytotoxicity, mutagenicity and cell transformation
H-Coal fuel oil	Higher nitrogen content	Higher NO_x emissions	Severely hydrotreated non-mutagenic, non-tumorigenic, low cytotoxicity
EDS fuel oil	—	Higher NO_x emissions	—
SRC II naphtha	Higher nitrogen, aromatics	—	Non-mutagenic, extremely low tumorigenicity cytotoxicity and fetotoxicity
H-Coal naphtha	Higher nitrogen, aromatics	—	Non-mutagenic
EDS naphtha	Higher nitrogen, aromatics	—	—
SRC II gasoline	Higher aromatics	—	—
H-Coal gasoline	Higher aromatics	—	—
EDS gasoline	Higher aromatics	—	—
Indirect Liquefaction			
FT gasoline	Lower aromatics; N and S nil	—	Non-carcinogenic
FT by-product chemical	—	N/A	—
Mobile-M gasoline	(Gross characteristics similar to petroleum gasoline)	—	—
Methanol	—	Higher aldehyde emissions	Affects optic nerve
Gasification			
SNG	Traces of metal carbonyls and higher CO	—	—
Low/medium-Btu gas	(Composition varies with coal type and gasifier design/operation)	(Emissions of a wide range of trace and minor elements and heterocyclic organics)	Non-mutagenic, moderately cytotoxic
Gasifier tars, oils, phenols	(Composition varies with coal and gasifier types, highly aromatic materials)	—	—

content of the synfuels (and the high arsenic content of the crude shale oil) can also be lowered to meet appropriate fuel specifications by the use of certain refining processes (for example, hydrotreating to reduce FBN). Another example of controlling undesirable product characteristics through process control (or in-plant treatment) is the elimination of traces of carbon monoxide and nickel carbonyl in SNG by proper operation of the methanator.

The data in Table 9 identify two products as highly hazardous because of mutagenic, tumorigenic, and cytotoxic properties. These are crude shale oil and fuel oils from coal liquefaction processes. These hazardous properties, which are characteristic of high boiling and tarry coal and petroleum materials, are caused by the presence of substances or classes of substances such as polycyclic aromatic hydrocarbons, hetero- and carbonyl-polycyclic compounds, aromatic amines and certain inorganics (for example, arsenic in crude shale oil).

In general, synfuel product characteristics that cause environmental concern in any wide-scale utilization scenario relate to the known or potential presence of toxic substances (including carcinogenic compounds associated with crude shale oil and heavy distillates from coal liquefaction and hazardous aromatics), fuel-bound nitrogen, volatile components, and minor and trace elements. Potential environmental concerns relating to anticipated product uses generally fall into three categories: occupational exposure, public exposure, and general environmental pollution. The occupational hazards affect workers manufacturing and using the products and personnel involved in facility maintenance and product distribution services. Public exposure primarily relates to air pollution resulting from product uses such as the use of gasoline in automobiles (affecting motorists at service stations), and hazardous fugitive emissions from storage tanks, product transfer points, leaks/spills, and product uses (for example, products produced from petrochemicals). In the general category of environmental pollution, major contributors would include accidental spills, sludges from product storage tanks and spill cleanups, and solid, liquid, and gaseous wastes associated with combustion and combustion-related air pollution control.

BASIS FOR PRIORITY RANKING OF SYNFUEL PRODUCTS

As noted previously, the objective of the study is to provide input to the EPA effort for: (1) assessing the environmental implications of a mature synfuel industry and of large-scale utilization of synfuel products; and (2) planning and prioritizing regulatory and research and development programs. Accordingly, a system was developed and used to rank the synfuel products from the standpoint of environmental concerns and to identify those products and areas of concern that should receive more immediate and greater regulatory and R&D attention. The ranking is based on the data presented previously and is subject to the limitations of the existing product characterization data and the assumptions used in developing the productions and use scenarios; the product rankings will most likely change as more data become available, especially for those products for which little or no data are currently available. It should also be noted that the specific approach used represents only one of many approaches that could be used to rank synfuel products from the standpoint of environmental concerns.

The product ranking system is based on:

- Reported or estimated environmentally significant characteristics of synfuel products relative to those of their petroleum analogs, based on considerations of exposure potential, combustive and evaporative emissions, toxic hazards, cost of control, and the extent of regulatory protections under key existing environmental legislations. Products for which the environmental risks and control needs are greater and for which less protections can be anticipated under existing regulations have been given a higher ranking.

- The estimated quantity of products used, both in absolute terms and as percentages of the total (synfuel and petroleum) used nationwide (Table 3)and regionally. The greater the amount of the product used and the percentage of usage, the greater the potential for presenting environmental hazards, and hence a higher positive ranking.

- Considerable scientific and engineering judgement. Because of the lack of a solid data base, heavy reliance had to be placed on the professional judgement of experts most familiar with the domestic energy supply and demand picture, synfuel production/refining technologies, expected environmental characteristics of synfuel products, applicable controls, and regulatory needs.

Two approaches were examined for ranking the synfuel products, based on: (1) the limited product characterization data currently available (Table 9) supplemented by engineering judgement where appropriate; and (2) the premise that in the absence of detailed characterization data, and unless the available data indicate otherwise, it would be reasonable to assume that a synfuel product would be more hazardous than its petroleum analog. The first approach was selected and used to develop product rankings.

Under the first approach, a synfuel product would not necessarily be considered more hazardous because of the mere lack of detailed characterization data. Instead, assignment of a more positive ranking to a product is supported by actual data or is based on strong indications of greater potential hazards. Under the first scenario, prioritization of regulatory and R&D activities does not have to await collection of additional data, which should proceed concurrently as a separate effort.

The second approach operates on the premise that if there is any room for error in ranking synfuel products, it would be more advisable to err on the safe side. This scenario asserts that, in the absence of detailed characterization data and strong evidence to the contrary, synfuel products by their very nature (new chemicals from a more "exotic" source) should be considered more hazardous. Under this scenario nearly all synfuel products would be given a positive ranking, thereby reducing a ranking system's usefulness as a guide in prioritizing regulatory and R&D activities. Acquiring detailed characterization data and not necessarily concentrating on products that are known to present greater environmental concern would be emphasized under the second scenario.

ATTRIBUTE RATING PROCEDURE

Table 10 presents the assessment of the environmental concerns for various synfuel products relative to their petroleum analogs on a "barrel-per-barrel" basis. As indicated by the headings in the table, the relative ranking considers potential for exposure, emission, toxic hazard, cost of control, and adequacy of existing regulations. A (+) ranking is assigned to a product for an environmental attribute if the product is judged to present greater environmental concern than the petroleum analog; a ranking of (0) indicates that the environmental concern would be similar to or less than that of the petroleum product. Factors considered in assigning ratings to each product for each environmental attribute along with some examples of product ratings are presented in Table 11.

PRODUCTS RANKING

Table 12 presents the results of synfuel products ranking. The products are ranked into three groups: those eliciting the most concern, ranked as "1"; those indicating "modest" concern, ranked as "2"; and those generating a "low" level of concern at the present time, ranked as "3". As noted in the table, in the near term (1980-1987 period), synfuel products of concern are primarily the shale oil products and medium-Btu gas and SNG from coal gasification. Shale oil refinery feed elicits the most regulatory attention; other shale oil products and medium-Btu gas elicit modest concern, and SNG requires a low level of attention.

For the 1988-1992 period, when products from SRC II and the F-T processes will also be marketed, the products eliciting the most concern would be shale oil refinery feed, fuel methanol, SRC II fuel oil, and gasifier tars and oils. F-T products and LPG from SRC II are ranked as low priority products during 1988-1992. During the 1993-2000 time frame, shale oil refinery feed, medium-Btu gas, gasifier tars and oil, and fuel oils from the three liquefaction processes are given "1" rankings; F-T products are assessed as "3", and all other products are given a "2" ranking.

The rankings generally indicate the greatest level of environmental concern and regulatory requirements for shale oil refinery feed and coal liquids. These liquids have been demonstrated to be more hazardous than petroleum crude and fuel oils (a major factor in assigning a "1" ranking). This and the fact that shale oil products will be the synfuels that are

TABLE 10. RELATIVE ASSESSMENT OF THE ENVIRONMENTAL HAZARDS ASSOCIATED WITH SYNFUELS PRODUCTS AND PETROLEUM ANALOGS

PRODUCT	EXPOSURE		EMISSION FACTOR		TOXIC HAZARD		Cost of Control	ADEQUACY OF EXISTING REGULATIONS			
	Transport & Storage	End Use	Transport & Storage	End Use	Transport & Storage	End Use		CAA	CWA	RCRA	TSCA
Crude shale oil (fuel)	+	0	0	+	+	+	+	+	+	+	0
Shale oil refinery feed	+	0	0	0	+	+	0	0	+	+	0
Shale jet fuel	0	0	0	+	0	+	+	+	0	+	0
Shale diesel fuel	0	0	0	+	0	+	+	+	0	+	0
Shale residuals	0	0	0	+	+	+	+	+	+	+	0
Shale gasoline	0	0	0	+	0	+	+	+	0	+	0
Low-/Medium-Btu gas (coal)	0	0	0	+	+	+	+	+	0	+	0
SNG (coal)	0	0	0	0	0	0	0	0	0	0	0
Gasifier tars and oils	0	0	0	+	+	+	+	+	+	+	0
Gasifier phenol	0	0	0	+	+	+	0	0	0	0	0
F-T LPG	0	0	0	0	0	0	0	0	0	0	0
F-T medium Btu gas	0	0	0	0	0	0	0	0	0	0	0
F-T SNG	0	0	0	0	0	0	0	0	0	0	0
F-T heavy fuel oil	0	0	0	0	0	0	+	0	0	+	0
F-T gasoline	0	0	0	0	0	0	0	0	0	+	0
M-gasoline	0	0	0	0	0	0	0	0	0	+	0
F-T diesel fuel	0	0	0	0	0	0	0	0	0	+	0
Fuel methanol	+	0	0	+	0	0	0	+	0	+	0
SRC II fuel oil	+	0	0	+	+	+	+	+	+	+	0
SRC II naphtha	0	0	0	0	+	+	0	0	+	+	0
SRC II LPG	0	0	0	0	0	0	0	0	0	0	0
EDS fuel oil	+	0	0	+	+	+	+	+	+	+	0
EDS naphtha	0	0	0	0	+	+	0	0	+	+	0
EDS LPG	0	0	0	0	0	0	0	0	0	0	0
H-coal fuel oil	+	0	0	+	+	+	+	+	+	+	0
H-coal naphtha	0	0	0	0	+	+	0	0	+	+	0
H-coal LPG	0	0	0	0	0	0	0	0	0	0	0

TABLE 11. FACTORS CONSIDERED IN ENVIRONMENTAL ATTRIBUTE RANKING (SYNFUEL PRODUCTS RELATIVE TO PETROLEUM/NATURAL GAS ANALOGS)

Attribute	Factors Considered	Example
Exposure/Transport and Storage	Potential for environmental contamination and public exposure from releases due to accidents, spills and fugitive emissions	(+) ranking for crude shale oil and direct liquefaction fuel oils because of higher content of water soluble compounds
Exposure/End Use	Potential for exposure due to end uses (e g , occupational exposure or exposure to combustion products)	(0) ranking for all products, products will be used in the same manner as petroleum products
Emission Factor/Transport and Storage	Amount of material released as a result of transport and storage activities (without regard to pollutant mobility and number of people potentially exposed)	(0) ranking for all products, no higher volatility or greater potential for accidental spills indicated
Emission Factor/End Use	Amount of pollutants released as combustive and evaporative emissions	(+) ranking for low-/medium-Btu gas due to higher emissions of trace elements and heterocyclics
Toxic Hazard/Transport and Storage	Potential for human and ecological toxicity in connection with transport/storage activities	(+) ranking for crude shale oil because of greater mutagenicity
Toxic hazard/End Use	Toxicity of combustive and evaporative emissions	(+) ranking for crude shale oil due to greater amounts of carcinogenic substances and higher emissions of NO_x when used as fuel
Cost of Control	Added control costs for regulated pollutants (especially NO_x)	(+) ranking for shale oil gasoline due to possibly more rapid deactivation of catalytic converter (e g , by arsenic and PNA's)
Adequacy of Existing Regulations		
Clean Air Act (CAA)	Potential emissions of hazardous substances other than pollutants covered by existing standards	(+) ranking for fuel methanol due to emission of aldehydes
Clean Water Act (CWA)	Estimated adequacy of available control technologies for wastewaters containing synfuel products	(+) ranking for direct liquefaction fuel oils due to estimated lower biodegradability
Resource Conversation and Recovery Act (RCRA)	Estimated hazards posed by synfuel wastes	(+) ranking for low-/medium-Btu gas due to estimatec more hazardous nature of sludges produced from air pollution control (when used as fuel)
Toxic Substances Control Act (TSCA)	Mandate of the act to regulate new products, new uses, or products produced using different processes presenting unreasonable risks	(0) ranking for all products, assuming adherence to the mandate of the Act

TABLE 12. PRIORITY RANKING OF SYNFUEL PRODUCTS FROM THE STANDPOINT OF ENVIRONMENTAL CONCERNS*

Product	1980-1987	1988-1992	1993-2000
Crude shale oil (fuel)	2	-	-
Shale oil refinery feed	1	1	1
Shale jet fuel	2	2	2
Shale diesel fuel	2	2	2
Shale residuals	2	2	2
Shale gasoline	2	2	2
Medium Btu gas (coal)	2	2	1
SNG (coal)	3	3	3
Gasifier tars & oils	-	1	1
Gasifier phenol	2	2	2
F-T LPG	-	3	3
F-T medium-Btu gas	-	3	3
F-T SNG	-	3	3
F-T heavy fuel oil	-	3	3
F-T gasoline	-	3	3
Mobil-M gasoline	-	3	3
F-T diesel fuel	-	3	3
Fuel methanol	-	1	1
SRC II fuel oil	-	1	1
SRC II naphtha	-	2	2
SRC II LPG	-	3	2
EDS fuel oil	-	-	1
EDS naphtha	-	-	2
EDS LPG	-	-	3
H-coal fuel oil	-	-	1
H-coal naphtha	-	-	2
H-coal LPG	-	-	3

*Degree of concern: most=1, modest=2, and low=3; - indicates product not produced or not used as indicated expected to first enter the market on a large scale, are the major factors that flag near-term environmental concerns for shale oil products in general and shale oil fuel and refinery feed in particular.

DATA LIMITATIONS AND RELATED PROGRAMS

As noted previously, there are a number of major gaps in the existing data base that preclude accurate analysis of the environmental concerns associated with a future large-scale utilization of synfuel products in the U.S. These gaps relate to: (a) present uncertainties regarding the size of the industry, specific synfuel technologies that will be used and product slates that will be produced, locations of production facilities and product distribution systems, and the specific areas of synfuel use; and (b) lack of adequate characterization data on synfuel products and on the analogous petroleum products that they will partially or totally replace. The first category of data limitations impacts the regional environmental implications and synfuel production scenarios and market analyses that were developed; whereas the second category of limitations introduces uncertainties in the estimated characteristics of synfuel products and the analysis of environmental concerns. Both types of data limitations impact the regional environmental implications and the ranking of the synfuel products.

At present, the first category of data gaps can only be partially filled (for example, through an engineering analysis to determine optimum product slates). Many of the gaps in the second category, however, can and should be filled through testing and evaluation of synfuel products obtained from existing U.S. pilot plants and commercial facilities abroad.

A number of chemical and biological/ecological testing programs are currently under way that are expected to substantially improve the quality of the existing data base on synfuel products. These programs are conducted and sponsored largely by DOE and EPA. In addition, a number of product performance testing efforts are under way or are planned that provide excellent opportunities for cost-effective collection of end use environmental data. These programs include testing shale-derived jet fuels in commercial and military aircraft engines (U.S. Air Force, Wright-Patterson AFB; U.S. Navy); standing diesel engine tests with SRC II and shale oil diesel fuels (DOE Bartlesville Energy Research Center); testing a spectrum of synfuel gasoline and jet fuels in ground and air transportation vehicles (U.S. Department of Transportation); and evaluation of the use of synthetic fuels in utility boilers (Electric Power Research Institute). EPA is currently exploring the possibility of joining these programs to simultaneously acquire environmental end use data.

CONCLUSIONS

- In the next 20 years significant quantities of synfuel products are expected to enter the marketplace and in certain regions a very high percent of the currently used products will be replaced by their synfuel-derived analogs.

- Based on gross characteristics, synfuel products appear to be similar to petroleum products, but detailed characterization data are not available for many of the synfuel and petroleum products with which to assess and compare their safety.

- Large-scale transportation, distribution, and end use of certain synfuel products (for example, heavy distillates derived from coal liquids and shale oil) can present significant threats to the environment and the public health.

- Essentially all synfuel-related environmental projects that are planned or currently under way relate to the design and operation of synfuel plants and not to the subsequent distribution and utilization of products. The present study constitutes the first attempt to focus attention on the potentially broad and far-reaching environmental implications of large-scale marketing and utilization of synfuel products.

- A number of major test and evaluation programs are planned or currently under way to assess the combustion characteristics and general performance of synfuels relative to those of petroleum products. These programs provide excellent opportunities for collecting the environmental data needed for assessing the relative safety of synfuel products, determining the adequacy of the existing control technologies, and identifying regulatory needs.

RECOMMENDATIONS

Based on the results and conclusions of the study, the following recommendations are offered:

- <u>More systematic approach to product characterization and testing</u>. Much of the currently available synfuel product characterization and testing data are fragmentary and cannot be correlated. The results generally do not cover all parameters of environmental interest and have been obtained in "isolated" studies using samples from different batches of products. Better coordination among various on-going and planned studies (perhaps through establishing a "test tracking" system that would promote exchanges of information among various studies) is recommended to avoid duplication of effort and to ensure generation of appropriate environmental data in a most cost-effective manner.

- <u>Collection of environmental data in conjunction with planned performance testing programs</u>. Several synfuel product performance testing efforts are being planned by various governmental agencies; it is most appropriate and timely to review these programs and take full advantage of opportunities for simultaneous collection of environmental data. Collection of environmental data, which can be correlated with product performance, in conjunction with a systematic product characterization effort (recommended above) can provide valuable, timely inputs to the evolution of the synfuel industry and would ensure that: (1) environmental considerations are included in the selection of processes, equipment, and product slates for commercial facilities; and (2) the drafting of specifications for synfuel products and new source performance standards for synfuel plants and emissions standards for facilities using synfuel products are based on the best available technical and engineering data.

- Consideration of end use environmental implications in the selection of the product slates and in the development of the synfuel industry. Synfuel processes and the subsequent refining operations can produce a range of products for a spectrum of end use applications. By proper selection of the refining steps (and the operating mode for some synfuel processes), the product slate can be altered to favor the production of those products that present fewer and more controllable end use environmental impacts. Studies should be undertaken to define the engineering and economics of selecting environmentally acceptable product slate possibilities for various synfuel technologies. In this connection, better coordination and exchange of technical data should be promoted among process developers, regulatory agencies and potential users and planners to ensure that process "specialization" from a product slate viewpoint is taken into account in synfuel commercialization programs.

- Compilation of characterization/performance data on analogous petroleum products. Because of the large-scale and widespread utilization of petroleum products, these products have generally come to be viewed by the public as environmentally innocuous. Accordingly, the specifications for petroleum products have primarily emphasized performance with little attention to environmental consideration. Very little data are available (or if available, have not been published) on potential pollutants and toxicological and ecological properties of many of the petroleum products to provide a baseline for assessing the safety of synfuel products. It is recommended that the potential sources of data on petroleum products be contacted in an effort to compile all available data and identify data gaps. It is also recommended that the synfuel product testing and characterization efforts recommended above include parallel testing of petroleum-derived analogs.