Session VI: PRODUCT-RELATED CONSIDERATIONS

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RISK ASSESSMENT OF SYNFUEL TECHNOLOGY†

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PREMANUFACTURE REVIEW OF SYNFUELS UNDER TSCA†

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ABSTRACT

The Toxic Substances Control Act (TSCA) requires manufacturers to notify EPA at least 90 days before they produce a new chemical substance for commercial purposes. Once notified, EPA has 90 days, extendable for good cause to 180 days, to review the chemical. During the review period, the Agency can act to prohibit or limit the manufacture, processing, or use of a new chemical substance where it finds that the information available on the substance is insufficient for a reasoned evaluation of its risks and that (1) the chemical may present an unreasonable risk to human health or the environment or (2) significant human or environmental exposure can reasonably be expected. Certain synthetic fuel products (including certain byproducts and intermediates) may be new chemical substances under TSCA and therefore potentially subject to premanufacture notice requirements. This paper outlines TSCA premanufacture notification requirements; it describes how "new" chemical substances are defined; and it discusses the types of data that might be provided to EPA with a premanufacture notice on a synfuel.

INTRODUCTION

The Toxic Substances Control Act (TSCA) of 1976 was the first Federal statute addressing commercial chemicals through all phases of their life cycle -- manufacture, processing, distribution in commerce, use, and disposal -- rather than specific uses of chemicals or particular media in which they might be found. A key feature of the act, which Congress passed in response to highly publicized incidents involving chemicals like PCB's, vinyl chloride, and BCME, was its focus on prevention. By giving EPA authority to require testing on suspected chemicals and by requiring it to review new chemicals before manufacture, Congress hoped to make it possible for the Agency to act against unreasonable risks before actual harm to human health and the environment occurred, rather than to address hazardous situations only after the damage had been done.

TSCA's premanufacture notice (PMN) requirements for new chemicals epitomize this preventive approach. Under §5, companies must notify EPA 90 days before they produce a new chemical, giving EPA the opportunity to review the chemical before exposure occurs. Synthetic fuels developers, because they will be manufacturing new fuels and related products, may in some cases be subject to these requirements. We recognize that this possibility has raised considerable concern in the synfuels industry.

Because of this concern, the EPA Office of Toxic Substances, which is responsible for administering TSCA, is committed to working with industry to clarify TSCA requirements and to ensure that premanufacture notice requirements do not unnecessarily delay the development of synfuels. Toward this end, we have met with several trade organizations and private companies to address both general and specific concerns, and we are cooperating with other offices in EPA and other government agencies to avoid duplication and to ensure a consistent approach. In carrying out our responsibilities under TSCA, we will be careful to avoid constructing artificial barriers to development -- that is, those that do not contribute to results with substantial health or environmental benefits.

In the remainder of this paper, we discuss in more detail TSCA's premanufacture notice requirements, the applicability of these requirements to synthetic fuels (in particular, coal-based fuels), and the types of data that manufacturers might develop in preparing a PMN.

SECTION 5 PREMANUFACTURE NOTICE REQUIREMENTS

Section 5(a) of TSCA requires companies to notify EPA at least 90 days before beginning to manufacture or import a "new chemical substance" for commercial purposes. As explained later, new chemical substances are defined under the Act as substances not listed on EPA's Chemical Substance Inventory, a compilation of chemicals in commercial production first published in 1979. Once notified, EPA has 90 days, extendable for good cause to 180 days, to review the potential risks likely to be posed by the new substance.

During the review period, EPA can act under §5(e) to prohibit or limit the manufacturing, processing, distribution, use, or disposal of the substance, pending the development of data, if it finds that the information available on the substance is insufficient for a reasoned evaluation of its health and environmental effects *and* that (1) the chemical *may present* an unreasonable risk to human health or the environment or (2) significant human or environmental exposure can reasonably be expected. If the Agency finds that the substance *will present* an unreasonable risk, it can regulate it under §5(f). When EPA does not take action under §5(e) or §5(f) during the review period, manufacture or import can begin without restrictions. After commercial manufacture begins, the substance is added to the inventory. At that point, the substance is no longer "new," and other manufacturers are free to produce it without submitting a PMN.

Section 5(d) of TSCA specifies the information that must be included in a PMN. In general, manufacturers must provide known or "reasonably ascertainable" information on chemical identity, anticipated production volume, categories of use, byproducts, workplace exposure, and manner or methods of disposal.* They are also required to provide test data that they have already developed and to describe any other information on health and safety they know or can "reasonably ascertain." However, TSCA -- unlike laws regulating the introduction of pesticides or drugs into commerce -- imposes no mandatory testing requirements for new chemicals.

The key to EPA's review of new chemicals under TSCA is the concept of "unreasonable risk." The Agency has not developed any general criteria for determining "unreasonable risk," because the finding depends too much on the specific situation. The Agency's approach to determining unreasonable risk, however, is illustrated in Figure 1. Potential toxicity (including ecotoxicity) and exposure define the risks a substance presents under specific circumstances of manufacture, processing, distribution, use, or disposal. To determine whether these risks are "reasonable," the Agency balances them against the benefits to be derived from the product, the cost of measures necessary to reduce risks, the availability of substitutes, and the comparative risks posed by products they may replace in the market.

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* Some of the information submitted in a premanufacture notice may be confidential, including highly sensitive business information. The Office of Toxic Substances routinely handles such information under TSCA, and it has established elaborate procedures (including serious penalties) to prevent its disclosure.

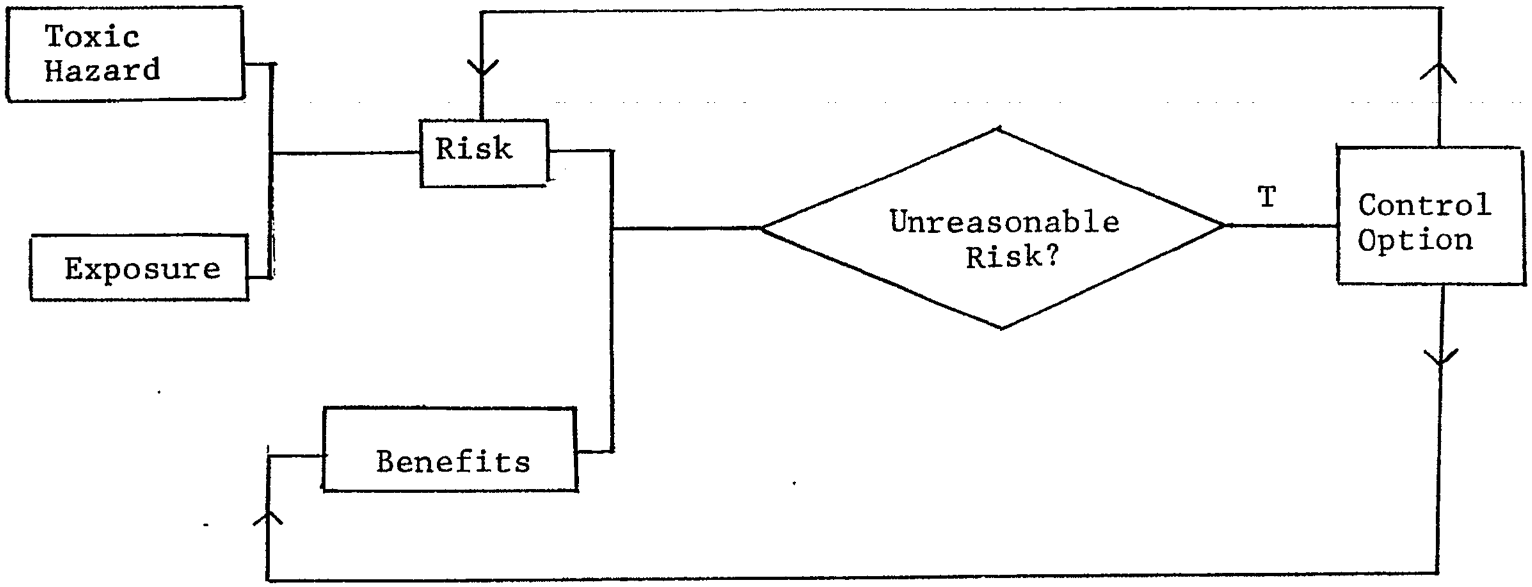

Figure 1. Determination of Unreasonable Risk Under TSCA

Several points about the review of new chemicals under TSCA §5 that are often misunderstood, particularly by companies more familiar with EPA permitting offices, should by now be clear. First, §5 imposes a notification requirement; it does not set up a licensing or registration program. To limit or halt production, EPA must take positive action against a chemical, based on certain specific findings. Otherwise, the chemical can enter commerce unregulated. Consequently, the Agency has in no sense "approved" a chemical that it has not regulated under §5. Second, TSCA does not impose testing requirements on manufacturers of new chemicals. Instead, the manufacturer of a new chemical has the responsibility to determine what level of testing, if any, is appropriate for a chemical, given its composition and projected uses. Finally, the "unreasonable risk" standard of TSCA incorporates the principle that the risks of a chemical can only be evaluated meaningfully within the context of the benefits derived from it and the costs of regulation. EPA's goal under TSCA is to balance these considerations rather than to reduce risk to some absolute "acceptable" level or to impose some other standard, such as best available technology.

To date, EPA has reviewed more than 800 new chemicals under the premanufacture review program. All these have been general industrial chemicals, such as intermediates, dyes, photographic chemicals, and lubricant additives. None has been a synthetic fuel. Therefore, it is difficult to make observations on synfuels and PMN requirements based on the history of the PMN program to date. Several special features of synfuels will distinguish them from new chemicals previously reviewed in the PMN program and raise particular issues for the PMN review process and for companies submitting notices. These features include:

- The national interest in alternate fuels development and energy independence
- The tremendous investments in synfuels development before commercialization
- The staged development of synfuel projects, which may include process and product changes in the course of commercialization, and therefore may complicate the task of characterizing the product and its toxicity
- The large production volume projected for synfuels, the potential for exposure to some commercial fuel products, and the presence of potentially toxic substances in some synfuel products

- The difficulties involved in evaluating health and environmental effects of complex, multicomponent substances like synfuels

- Public concern about potential hazards from synfuels

Because of the importance of synfuels projects and the money committed to them, developers subject to PMN requirements are encouraged to consult EPA well before PMN submission to ensure that they are developing information sufficient for a reasoned evaluation of risk. In this way, EPA and industry can ensure that the PMN process will not unecessarily delay the commercialization of a product.

PMN REQUIREMENTS AND SYNFUELS

Some synfuels developers -- and companies refining new synfuels -- may be intending to make products that would be "new chemical substances" subject to TSCA premanufacture notice requirements. OTS is now reviewing the applicability of §5 requirements to synfuels (for example, how the research and development exemption of §5(h)(3) should apply to projects of this scale), and it is developing a consistent approach to defining and characterizing synfuel products, so that industry can readily determine whether a specific product is new. Although this work is not yet completed, it is possible at this point to provide developers some preliminary guidance on the Office of Toxic Substances' current thinking on premanufacture notice requirements for synfuels. For more specific guidance, we recommend that individual developers consult the Office.

WHEN IS A PMN REQUIRED?

The PMN Requirement Is Substance-Specific

"Chemical substances" have a special definition under TSCA -- the term covers both discrete chemical compounds (e.g., benzene or sodium chloride) and complex substances produced by chemical reaction (e.g., coal tar or slag), including refined products (e.g., petroleum distillates). However, the term excludes "mixtures" that could be produced for commercial purposes by combining substances without a chemical reaction. Complex materials such as typical coal liquids are not considered "mixtures" under TSCA, but rather are chemical substances, because they could not practicably be made by mixing their constituents.

TSCA premanufacture notice requirements apply to such "substances" if they are new. In this respect, these requirements differ from permitting requirements, which apply to facilities rather than chemicals. A new facility producing "existing" substances would not be subject to PMN requirements. On the other hand, a single facility is likely to produce several products, any or all of which might be "new" and therefore subject to PMN.

"New" Chemical Substances Are Chemicals Not Listed on the TSCA Chemical Substance Inventory

Under §8(b) of TSCA, EPA has compiled and keeps current an inventory of chemical substances in commerce, first published in June 1979. Chemicals listed on the inventory are considered "existing" substances, not subject to PMN notice requirements. When chemicals complete PMN review and enter commercial production, they are added to the inventory. Therefore, manufacturers may determine whether their substances are new by consulting this list or, where questions of product identification are difficult, by asking the Office of Toxic Substances whether the substances are listed.

The Substance Must Be Manufactured or Imported "For Commercial Purposes"

TSCA §5 requirements specifically apply to chemical substances manufactured "for commercial purposes." This includes intermediates and other chemicals consumed entirely on the site at which they are manufactured. As a result, intermediate streams used in making new synthetic fuels may be subject to PMN requirements, even if they are never sold or distributed in commerce.

Research and Development Chemicals Are Exempt From PMN Requirements

Chemicals manufactured "only in small quantities" solely for research and development are specifically exempted from PMN requirements by §5(h)(3) of the Act. Activities falling within the category of R&D include the evaluation of the physical, chemical, production, and performance characteristics of a substance. Thus, pilot plant operations designed to assess manufacturing or refining processes, test burns to evaluate fuel efficiency or emissions, and other product characterizations are possible without a PMN. These evaluations may be carried out by people other than the manufacturer, including potential industrial customers. Furthermore, the sale of a product to a potential customer who will use it only for R&D does not remove the product from the category of R&D. EPA has not placed a specific volume limit on the R&D exemption, but rather has stated that "only in small quantities" means only in quantities no greater than reasonably necessary for R&D (see 40 CFR 710.2(y)). For synfuels, because of the nature of R&D activities, "small quantities" may be large compared to production volumes for typical industrial chemicals.

Nonisolated Intermediates Are Exempt

Chemical intermediates not intentionally removed from the equipment in which they are manufactured are exempt from PMN requirements. (See 40 CFR 710.4(d)(8).) As a result, nonisolated process streams in a synfuels plant are not subject to these requirements. However, if the intermediate stream is removed from the plant equipment -- including for storage -- it may be subject.

Some Commercial Byproducts Are Exempt

The inventory reporting rules exempt from PMN requirements byproducts that have commercial value only to organizations who (1) burn them as fuel, (2) dispose of them as waste, including in a landfill or for enriching soil, and (3) extract component chemical substances from them. (See CFR 710.4(d)(2).) Under this provision, certain byproduct streams burned for process heat as an alternative to disposal may be exempt from PMN require ments -- for example, phenols produced as a byproduct of coal gasification would not be subject to PMN if incinerated.

HOW CHEMICAL SUBSTANCES ARE DEFINED

When EPA compiled the initial TSCA inventory, it faced a number of complex issues related to chemical identification and nomenclature. The resolution of these issues, reflected in the way products were reported for the inventory and how they are listed, now defines the Agency's approach to defining products for PMN purposes.

For single-component substances that can be characterized by a molecular formula -- like ammonia, benzene, and methanol -- the problem of identification was simple. These products are listed on the inventory under their chemical names; manufacturers of the substances, therefore, are not subject to PMN requirements, regardless of how the substances are made and what levels of impurities they contain.

Complex reaction products -- for example, materials produced in coking coal or refining petroleum -- presented a very different problem. Here, the products could not be defined by a single structure or an unambiguous chemical name. Instead, these products were defined by source material and process of manufacture rather than by compositional data alone. An attempt was made to define product categories broadly enough so that limited variations in source (e.g., substitution of one grade of coal or one petroleum crude for another) or slight changes in process did not create a new product, but at the same time narrowly enough so that substances within a product category could be expected to be similar in composition and biological activity.

This approach can best be illustrated by the listing of refined petroleum products on the inventory. For example, the inventory entry "light hydrocracked distillate (petroleum)" is defined as "a complex combination of hydrocarbons from the distillation of the products of a hydrocracking process. It consists primarily of saturated hydrocarbons having carbon numbers predominantly in the range of C_{10} through C_{18}, and boiling in the range of 160°C to 320°C." This description, it can be seen, identifies the source material (petroleum), the process of manufacture (hydrocracking and distillation), and composition (C_{10}-C_{18} saturated hydrocarbons) as well as a physical property (boiling range) that roughly correlates with chemical composition. Any hydrocarbon product that met these criteria would be considered the same product for inventory purposes and therefore would not be subject to PMN. Comparable products from a different source material or manufactured by a different process, however, would be different chemical substances under the inventory rules. (Other examples of petroleum products are given in Table 1.)

This discussion should make it clear that, for TSCA inventory purposes, coal-derived synthetic fuels are, a priori, different chemical substances from petroleum-based fuels. An inventory entry for petroleum naphtha, for example, would not cover a naphtha derived from coal, even if the general composition and the boiling range of the products were similar, because their source materials are different. In the same way, a naphtha derived from coal gasification is not comparable to a naphtha derived from the solvent-refining of coal, because of the clear difference in process. Therefore, a PMN might be required for a naphtha produced in a high-Btu coal gasification operation even though petroleum naphtha and coal naphtha produced by pyrolysis were listed on the inventory. (However, we recognize that at some point in refining coal, oil shale, and petroleum products becomes so similar that source should no longer be a factor in product definition.)

The Office of Toxic Substances is now working to develop product definitions for synfuels comparable to definitions

TABLE 1. SAMPLE PETROLEUM PRODUCT DEFINITIONS ON THE TSCA CHEMICAL SUBSTANCE INVENTORY (FROM TOXIC SUBSTANCES CONTROL ACT)

CRUDE OIL DISTILLATION STREAMS

Light Straight Run Naphtha (Petroleum) [*64741-46-4]

A complex combination of hydrocarbons produced by distillation of crude oil. It consists predominantly of aliphatic hydrocarbons having carbon numbers predominantly in the range of C_4 through C_{10} and boiling in the range of approximately minus 20°C to 180°C (-4°F to 356°F).

Heavy Straight Run Naphtha (Petroleum) [*64741-41-9]

A complex combination of hydrocarbons produced by distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C_6 through C_{12} and boiling in the range of approximately 65°C to 230°C (149°F to 446°F).

Straight Run Kerosine (Petroleum) [*8008-20-8]

A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C_9 through C_{16} and boiling in the range of approximately 150°C to 290°C (320°F to 554°F).

Straight Run Middle Distillate (Petroleum) [*64741-44-2]

A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C_{11} through C_{20} and boiling in the range of 205°C to 345°C (401°F to 653°F).

Straight Run Gas Oil (Petroleum) [*64741-43-1]

A complex combination of hydrocarbons produced by the distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C_{11} through C_{25} and boiling in the range of approximately 205°C to 400°C (401°F to 752°F).

OTHER PRODUCTS

Light Hydrocracked Distillate (Petroleum) [*64741-77-1]

A complex combination of hydrocarbons from the distillation of the products from a hydrocracking process. It consists predominantly of saturated hydrocarbons having carbon numbers predominantly in the range of C_{10} through C_{18}, and boiling in the range of approximately 160°C to 320°C (320°F to 608°F).

Hydrotreated Light Distillate (Petroleum) [*64742-47-8]

A complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C_9 through C_{16} and boiling in the range of approximately 150°C to 290°C (302°F to 554°F).

Light Catalytic Cracked Distillate (Petroleum) [*64741-59-9]

A complex combination of hydrocarbons produced by the distillation of products from a catalytic cracking process. It consists of hydrocarbons having carbon numbers predominantly in the range of C_9 through C_{25} and boiling in the range of approximately 150°C to 400°C (302°F to 752°F). It contains a relatively large proportion of bicyclic aromatic hydrocarbons.

Crude Phenolic Compounds (Petroleum) [*64743-03-9]

A complex combination of organic compounds, predominantly phenol, cresols, xylenols and other alkylated phenols obtained primarily from cracked naphtha or distillate streams by alkaline extraction.

Vacuum Residuum (Petroleum) [*64741-56-6]

A complex residuum from the vacuum distillation of the residuum from atmospheric distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly greater than C_{34} and boiling above approximately 495°C (923°F).

already developed for petroleum products. The goal is to divide the spectrum of potential synfuel products into generic chemical substance categories that will be unambiguous both to industry and EPA and that will reflect likely compositional differences. This scheme would define how new synfuels would be listed on the inventory. As a result, it would make it possible to determine which products should be considered equivalent to existing products for PMN purposes and might be subject to PMN requirements. Specifically, OTS is addressing questions like: Are products from different coal liquefaction processes (e.g., SRC-II, EDS, and H-coal) likely to be sufficiently similar in composition and biological activity to justify their treatment as the same substance for inventory and PMN purposes? (In other words, if an SRC-II liquid is entered on the inventory, would a comparable EDS or H-coal product automatically become an existing substance not subject to PMN?) At what point in the refining process should synfuel products be considered essentially equivalent to comparable petroleum products and therefore not be subject to PMN requirements? In this work, OTS has solicited information and advice from the American Petroleum Institute, and it is in contact with the National Council on Synthetic Fuels Production. The Office is also willing to meet with other organizations or individual companies who have an interest in these questions.

Until this work is completed, it is difficult to provide definitive answers to questions about whether one synfuel product should be considered equivalent to another for PMN purposes, or how many synfuels are likely to be subject to PMN requirements. It is possible, nevertheless, to provide some guidance on requirements for certain specific products. For example:

1. Sulfur, ammonia, and carbon dioxide produced in the gasification or liquefaction of coal are existing substances and thus are not subject to PMN requirements.

2. Methanol produced from coal is equivalent to methanol listed on the inventory and thus is not subject to PMN. However, indirect coal liquids are not on the inventory and therefore may be subject to PMN requirements if manufactured for commercial purposes.

3. Substitute natural gas produced by coal gasification is predominately methane, which is listed on the inventory, and therefore is not subject to PMN.

4. SRC I wash solvent, SRC I mineral residue, and SRC naphtha, which are listed on the inventory, are not subject to PMN requirements. Other SRC products reported

for the inventory are under review by OTS, as described below.

Because of the complexity of product definitions, we encourage synfuel developers to consult OTS on the applicability of PMN requirements to their products.

STATUS OF SYNFUELS REPORTED FOR THE INVENTORY

Under the previous administration, OTS began a review of 20 synfuel products (9 SRC products and 11 oil shale products) reported for the inventory to determine if they should have been included on the list. The key question was whether the products had been manufactured for purposes other than research and development during the period when the inventory was compiled. OTS has determined that certain of the products -- including the SRC products listed under item number 4 above -- had in fact been properly listed. For the other products, OTS decided that it did not have enough information to make a determination, and it asked for further information from the companies that had reported them for the inventory. We anticipate that the Agency will decide the status of these products in the near future.

PMN SUBMISSIONS

As previously discussed, TSCA requires PMN submitters to provide certain information on chemical identity and exposure, but it does not require manufacturers of new chemical substances to develop health and safety data specifically for their notices.* However, §5(e) gives EPA the authority to delay the commercial production of a new chemical in the absence of data necessary for a reasoned evaluation of the chemical's health and environmental effects -- if the substance "may present an unreasonable risk" or that there will be "significant or substantial exposure" to it.

The nature of this §5(e) authority, and EPA's interpretation of it, has raised concern among some prospective synthetic fuel producers. Several companies have asked OTS to identify the data

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* For general guidance on EPA's interpretation of premanufacture notice requirements, see Toxic Substances Control: Premanufacturing Notification Requirements and Review Procedures; Statement of Interim Policy (44 FR 28564, May 15, 1979) and Toxic Substances Premanufacture Notification Requirements and Review Procedures: Statement of Revised Interim Policy (45 FR 74378, November 7, 1980).

it would consider sufficient for a "reasoned evaluation" of a particular synfuel and to comment on the appropriateness of specific test plans. To address such questions, the Agency has established a Synfuels/Toxics Workgroup, managed by OTS, which can provide guidance to individual producers and will facilitate the review of PMN's on synfuels. Synfuels developers are encouraged to discuss questions concerning data development and methods of controlling risks with this group before submitting a PMN.

Because there are no testing requirements under TSCA for new chemicals, EPA has not developed prescriptive guidelines for data development on synfuels. In addition, it is difficult to define a single approach for different products because, among other reasons, the specific composition of a product and the conditions of its production and use will influence how much and what types of information might be appropriate. However, we believe that the following general principles are applicable to any program evaluating risks from synthetic fuels:

- Data should be appropriate to what is known about chemical composition and exposure. For example, if exposure is limited, limited data may be sufficient for a reasoned evaluation.

- Full characterization of risks before a synfuel is manufactured commercially may in some cases be infeasible. Although the amount of data available may be limited early in commercial development, concern for risk posed by a substance would be limited by the fact that exposure and production volume are relatively low. However, as a substance grows in the market, more data might in some cases be appropriate.

- New synthetic fuels should be evaluated in comparison to the petroleum products they would replace to provide a perspective on the risks they might present. If replacing petroleum products by a synfuel will not lead to an increase in risk, risks from the new synfuel should generally be considered reasonable.

In the remainder of this presentation, we will describe in somewhat more detail the kinds of thinking that typically goes into a risk evaluation and that lies behind OTS' general approach to assessing data provided in a PMN.

CHEMICAL CHARACTERIZATION

In many cases, the chemical composition of a product -- including the extent to which it contains minor constituents of known or suspected toxicity, like aromatic amines, heterocyclic nitrogen compounds, and PNA's -- can serve as an important guide in determining what data are appropriate for evaluating risks. For example, a chemical analysis of a gasoline derived from indirect liquefaction might show that it was less aromatic and more aliphatic than typical petroleum gasolines, and contained a considerably lower level of toxicologically significant constituents. This could provide a rationale for limiting the extent of toxicity testing. At the same time, extensive testing of substances known to be highly hazardous may be redundant. For example, if a coal-derived residual fuel contained significant quantities of known or suspected carcinogens, the premanufacture review of this substance would focus on potential exposure and the manner of uses to establish that risks are adequately controlled.

EXPOSURE ASSESSMENT

Conditions of exposure are also an important factor in deciding what health and environmental-effects data would be appropriate to evaluate risks posed by a specific substance. Typically, exposure assessments address direct exposure to humans, indirect exposure to humans from environmental release, and exposure to the environment during all phases of a substance's life cycle -- manufacture, handling, distribution, storage, and end use. Anticipated production volume for different uses, potential targets of exposure, and magnitude of exposure are also factors that often guide data development. We recognize that there is no simple formula for translating such considerations into a testing strategy. However, in reviewing PMN's on new chemicals, the Agency evaluates the data presented in the light of exposure-related considerations.

It is possible to illustrate in general terms how different exposure scenarios might influence data development. The following uses, for example, would on the whole reflect increasing levels of direct human exposure: industrial boiler fuel, diesel transport fuel, and consumer gasoline. EPA's review of health and environmental effects data on products within each of these categories would consider the different levels and modes of exposure -- where exposure is likely to be higher, data should provide greater certainty that a substance does not present an unreasonable risk. As a second example, tentative or preliminary data might be reasonable for products made in early-term plants, if the products would be used in a restricted or controlled manner.

EXISTING DATA

The Department of Energy, EPA, private companies, and other organizations have developed a considerable amount of information relevant to risks that may be posed by new synfuels. This includes data on the toxicity of comparable petroleum and synfuel products, exposure information on different fuel uses, information on the use of specific toxicity tests for complex mixtures like synfuels, toxicity data on chemicals likely to be found in a synfuel, and similar information. PMN submitters should consider the implications of this information in determining what and how much data they should develop.

TOXICITY AND ENVIRONMENTAL EFFECTS TESTING

As we stated before, TSCA does not require the testing of new chemicals. In addition, because the review of risks posed by a new synfuel will depend on the specific product and its projected uses, it is impossible to develop prescriptive guidelines for health and environmental effects data. Instead, synfuels developers are encouraged to discuss their products and testing plans with the Office of Toxic Substances before PMN submission.

OTS recognizes that the scale and scheduling of many synfuel projects are likely to make it difficult for developers to provide final health and environmental-effects data sufficient for evaluating risks associated with a full-scale commercial operation at the time they submit a premanufacture notice. For example, if a manufacturer is conducting long-term tests, results might not be available at the time of notice submission. In addition, products are likely to change in scaleup or as a result of process changes; in some cases, pilot-plant material available for toxicity testing may not be comparable to products later made in a commercial plant. Thus, if tests are being conducted on early-stage products, the relevance of the results of these tests to an evaluation of the potential effects of final commercial products should be considered. In such circumstances, technical judgment can be used to evaluate whether the final product is likely to present more or less of a problem than the tested material.

EPA understands that it is often common for the development of data to proceed as technology develops and commercial samples become available. It is possible, of course, that a commercial substance might later prove to be more hazardous than initially believed, or that subsequent data might show that the substance would present an unreasonable risk under certain circumstances. Companies developing a new product would typically have contingency plans for controlling exposure in this situation. These plans, for example, might call for restricting uses; imposing engineering controls; upgrading the product; changing the process or product slate; or similar measures. In reviewing PMN's on new synfuels, EPA will consider all these factors in assessing the reasonability of risk.

By early consultation with EPA about PMN-related issues, synfuels developers can ensure that PMN requirements do not unnecessarily delay the commercialization of their products, and that any differences on appropriate data development are resolved before formal PMN submission.

CONCLUSION

The evaluation of risks posed by synthetic fuels raises a number of complex issues. We cannot expect to achieve perfect certainty in this area, nor can we hope to eliminate all risk. Instead, EPA's standard under TSCA is "unreasonable" risk, which takes into account potential benefits, availability of substitutes, and risks posed by comparable products in society. Under §5, EPA has the responsibility to review new chemicals according to this standard before they enter commercial production. However, we recognize the unique issues raised by the premanufacture review of synfuels. Where PMN requirements apply to new synfuels, the Agency will work with developers to ensure that these requirements do not unduly impede technological innovation, while protecting health and the environment from unreasonable risk.

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METHANOL AS A CLEAN MAJOR FUEL

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ABSTRACT

The objective of this investigation of methanol as a major fuel was to provide perspective for officials of the U.S. Environmental Protection Agency's Industrial Environmental Research Laboratory at Research Triangle Park regarding possibilities for commercialization and the environmental implications associated with wide use of methanol as a substitute for petroleum-derived fuels.

It is recognized that the future of methanol fuel will ultimately be determined by economics. To gain widespread acceptance, methanol will have to be cheaper than competitive fuels after all advantages and disadvantages have been considered. No attempt is made here, however, to assess the competitiveness of methanol fuels at present prices for crude oil or to project the price at which they could be competitive. Such evaluations would be far beyond the scope of the study. Instead, the methanol fuels are considered relative to other fuels that might be used if an effort is launched to apply available technology to displacement of petroleum fuels as soon as possible. The major factors considered are:

1) Potential environmental consequences of introducing methanol.

2) Status of development of methanol fuel technology.

3) Cost and efficiency of synfuel processes.

4) Potential markets.

5) Prospects for commercialization of methanol fuels.

The intent is to develop an overview perspective by identifying all important factors in each category and presenting enough quantitative data to permit relative comparisons, without excessive detail.

BACKGROUND

At present there is concern over the rate of progress in development of advanced coal conversion processes for a synthetic fuels industry. One of the principal impediments is the inflation associated with a cost-spiral driven by continuing increases in the cost of oil and other fuels, including coal.

Because of the inflationary trend, many believe that plants that could be built now to use available technology will be cheaper to operate than plants built later to use improved processes that might come onstream in a few years. Also there is a continuing concern over America's continuing dependence on foreign oil. These factors have combined to create interest in utilizing immediately applicable coal conversion technology.

The only proven coal conversion technology is indirect liquefaction; that is, the conversion of coal to synthesis gas and subsequent conversion of this gas to liquid fuel. The proven routes for coal conversion include (1) the Fischer-Tropsch process, which converts synthesis gas directly to gasoline and other byproducts, and (2) a number of catalytic processes, which convert synthesis gas to methanol. Although the Fischer-Tropsch process has the advantage of producing gasoline directly, it has the disadvantage of producing many coproducts and byproducts, which must be marketed. Methanol may be used directly, as a premium fuel, in some applications, but may have to undergo subsequent conversion to gasoline, at some added cost, for use as a transportation fuel.

If a decision is made to build synthetic fuel plants with presently available technology, the Fischer-Tropsch process and methanol fuel processes will likely be used. The Fischer-Tropsch products are essentially the same as petroleum-derived fuels, so that their introduction into commerce would not require significant adjustment. In contrast, the introduction of methanol as a major fuel would require significant adjustment.

METHANOL AS FUEL: ENVIRONMENTAL IMPLICATIONS

Although some testing has been carried out to evaluate the use of methanol as a major fuel for automobiles and stationary sources, work to evaluate the potential environmental effects has not been extensive. Whereas some properties of methanol make it attractive as a fuel, others present problems. Experimental work to date has been encouraging, but many questions remain unanswered. Following are some of the more important environmental considerations.

1) Methanol has a lower flame temperature than petroleum-derived products. It also has wide limits of combustibility. These properties combine to make either automobiles or stationary sources that are designed for methanol fuels relatively lower emitters of nitrogen oxides.

2) Methanol combustion is essentially particulate-free. No carbon-to-carbon bonds are present to promote soot formation, which is associated with burning of petroleum-derived fuels.

3) Because sulfur in the feedstocks for methanol is removed in processing, combustion of methanol generates virtually no sulfur emissions.

4) Because of its high octane rating, methanol can be used in motor vehicles without additives, eliminating the emissions associated with additives to petroleum-derived fuels.

5) Methanol's low heat content (about half that of gasoline on a volumetric basis) necessitates the use of twice the volume and over twice the weight of fuel when it is substituted for gasoline or distillate oil.

6) Some methanol properties such as corrosivity, toxicity, and explosivity call for careful consideration. Although they have not caused problems in the closely controlled situations where methanol has been used as a commercial chemical, they must be given careful attention if it is widely used as a major fuel.

7) Other environmental considerations that have not been evaluated are the reactivity, persistence, and sensory detectability of methanol in the environment. These factors could be of great importance for a chemical with potential for release in large amounts to the environment, as illustrated by the experiences with oil spills. The high solubility of methanol in water suggests that spills of methanol would not persist as oil spills do. On the other hand, the contamination of lakes or major rivers with a toxic material that disburses into water could cause fish kills and also could produce water contamination that would not be readily detected without special precautions.

The most extensive body of experimental work on methanol as a fuel has dealt with its use as a gasoline substitute. Most attention has been given to methanol-gasoline mixtures, but consideration has also been given to the use of 100 percent methanol fuel for automobiles. Although it has been established that methanol could be substituted for gasoline, there is considerable controversy over advantages and disadvantages of doing so. Some researchers expect that methanol will give higher efficiency, improved performance, and reduced pollution.[1] Others claim the opposite on all or some of these points.[2,3] It is generally accepted, however, that the use of methanol in engines designed to take advantage of its high octane and unusual combustion characteristics would give performance as good as, or superior to that of gasoline on an equivalent Btu basis.

Experimental work with methanol as a fuel for use by stationary sources has been encouraging. Tests in which methanol fuel was fired in a utility boiler designed to burn natural gas or distillate oil showed methanol to be a superior fuel.[4] Concentrations of pollutants in the combustion gases were very low (no particulates, no sulfur oxides, and low nitrogen oxides). Also, the methanol fuel burned efficiently with a stable flame, and carbon previously deposited by oil burning was burned off of heat transfer surfaces with a resultant improvement in heat transfer. Tests of methanol fuels in commercial combustion turbines were also promising. Performance was excellent, and nitrogen oxide emissions were lower than those produced by firing natural gas. Studies of methanol as a turbine fuel for combined-cycle plants were also promising, and it has been suggested that such plants could be designed to be virtually pollution free.[5]

Consideration of methanol as a fuel for nonutility stationary sources led to the conclusion that it could replace distillate oil in home heating and would give increased efficiency. This study also concluded that methanol fuels could replace gas or distillate oil in commercial and industrial applications if due consideration is given to potential problems associated with its toxicity and flammability.[6]

In summary, past work indicates that methanol has potential for wide use as a high-quality environmentally attractive fuel. The studies also show clearly, however, that its use as a fuel will require special measures for environmental protection.

STATUS OF DEVELOPMENT FOR METHANOL FUEL PRODUCTION PROCESSES

All of the technology necessary to produce methanol for fuel use is proven. At present chemical-grade methanol is produced in amounts estimated at 30,000 ton/day. Most is produced from synthesis gas made from natural gas. The largest plant in operation today is a 2500-ton/day single-train plant, which has been operational for 10 years. Plants twice this large are now considered feasible. It is claimed that because of reduced quality requirements and improvements in technology, a 5000-ton/day plant for production of fuel-grade methanol would be only slightly larger than the operating plant producing 2500 ton/day. It is further suggested that methanol fuel plants should consist of 5 trains of 5000 ton/day each in capacity.[7]

Technology for production of synthesis gas from coal is also being applied widely outside of the United States. Lurgi and Koppers-Totzek coal gasifiers are the most discussed for use in commercial production of liquid fuel from coal. Both types have a long history of application in service of the general type required for production of methanol fuels, and both have been incorporated in planned installations.

The development of the Mobil-M process, which is said to convert methanol to gasoline with an efficiency of 95 percent, may be the key to avoidance of distribution and handling problems that might otherwise impede the application of methanol fuel technology.[8] The process was announced in 1976. Since then a 4-bbl/day pilot plant has been operated. Economic comparisons with commercially established Fischer-Tropsch units are claimed to show that the Mobil process is the most promising route from coal to gasoline.[9] Construction of a plant to convert methane-derived methanol to 12,500 bbl/day of gasoline is expected to begin in late 1981 in New Zealand. The plant, to be completed in the mid-1980's, will supply an estimated 1/3 of that country's transportation fuel.

Although all major components for production of methanol fuel from coal are proven technology, no plant has yet been built. Construction of such a plant would involve making the connection between coal gasifiers producing synthesis gas and methanol plants for the first time. Also, economy of scale would require the design of methanol trains larger than any yet built. And coal would be gasified on a scale unprecedented except in South Africa, where the "Sasol I" plant employing Fischer-Tropsch technology has operated since 1955. This plant employs thirteen gasifiers, each 12 feet in diameter. Proposed plants will be even larger. Sasol II, which came on stream recently, employs 36 gasifiers.[10] The problem associated with adaptation of processes and large scale operation should not present serious technical problems, but any element of risk has potential for making investors cautious about investing in multi-billion dollar plants.

COST AND EFFICIENCY OF METHANOL FUEL PROCESSES

The attractiveness of methanol fuels over fuels from alternative processes will depend primarily on cost. The thermal efficiency of the conversion process will be an important factor in the final production cost. Comparisons of both cost and efficiency of alternative production routes are complicated by the dependence of both on the quality of feed materials and the markets for potential products and coproducts. This is illustrated in Table 1, which shows a comparison of plants employing Lurgi gasification for production of methanol, Mobil M-gasoline, and Fischer-Tropsch synthesis, with and without, coproduction of SNG.[11] The column for efficiency shows the percentage of the input Btu that comes out as product. The last column shows investment cost in dollars per million Btu output per year. The lower efficiency and higher cost shown where SNG is not a product reflect losses associated with conversion of methane formed in gasification to synthesis gas for conversion to additional liquid product.

Table 1. Efficiency of Investment Cost Indirect Coal Liquefaction[11]

	Efficiency, %	Investment Cost, $\$/10^6$ Btu/yr
Methanol from Syn Gas		
Methanol	50.8	28.2
Methanol + SNG	60.4	21.8
Methanol - Mobil M		
Gasoline	48.7	34.3
Gasoline + SNG	58.2	24.0
Fischer-Tropsch		
Gasoline + diesel	35.7	45.3
Gasoline + diesel + SNG	50.8	25.2

The cost of production of liquid fuels is frequently given in dollars per million Btu in all products. Because this approach fails to account for differences in the value of the end products, however, it can give a distorted perspective of the potential for a given technology to satisfy present needs. Also, costs are often compared without due consideration of uncertainties attributable to stage of development. One recent study, however, generated data that give some feeling for the importance of these uncertainties in comparison of technologies.[12] Data from that report are shown in Table 2. The confidence index in Column 1 has two components: a letter indicating stage of development and a number indicating the estimated reliability of the cost. The energy cost is based on the total energy value for all products. The "reference price" is based on Btu outputs, adjusted downward in proportion to their value relative to gasoline for all products that are less valuable.

Data such as these must be considered approximations subject to variation not relating to the skill or objectivity of the estimators. They do, however, highlight several important points that are creating pressure to use presently available technology as a basis for beginning the development of a synthetic fuels industry:

1) Fischer-Tropsch and methanol fuels are more costly than new processes are expected to be. The estimated costs, however, are more reliable (as indicated by the confidence index) than those for the four developmental processes.

2) The cost advantages of developmental processes are not great. Unforeseen circumstances or inflation during the developmental period could cause them to be more expensive than plants that could be built now.

3) When credits are applied for quality of product, the relative economics change significantly. The net result is that methanol shows the lowest reference price and a confidence index better than that for any other process except Fischer-Tropsch.

TABLE 2. COST COMPARISON FOR ALTERNATIVE PROCESSES FOR PRODUCTION OF LIQUID FUELS FROM COAL[12]

	Confidence index*	Energy cost, $\$/10^6$ Btu	Reference price, $\$/10^6$ Btu
Fischer-Tropsch	A-2	4.99	5.52
Methanol	A-2	4.32	4.54
Mobil M-Gasoline	C-3	4.84	4.91
Exxon donor solvent	C-3	3.96	5.40
H-coal	C-2	3.58	4.81
SRC II	B-4	3.62	5.59

* Confidence index factors:

Process development	Economic reliability
D - Exploratory stage - not beyond simple bench tests	4 - Screening estimate, very approximate
C - Development stage - operated on small integrated scale only	3 - Incomplete definition for estimates used
B - Pre-commercial - successful pilot plant operation	2 - Firm basis for values developed
A - Complete - process demonstrated sufficiently to insure commercial success	1 - Values considered to be satisfactory for commercial venture

It is not intended to suggest that these data indicate superiority of any given process. Many situation-specific factors (type of coal, markets served, transportation modes available) will influence process selection for commercial projects. The results do, however, illustrate the potential advantages of applying available technology now.

POTENTIAL MARKETS FOR METHANOL FUEL

Methanol fuels have been demonstrated in a variety of applications:

1. Fuel for motor vehicles, alone, or in combination with gasoline.
2. Fuel for electric utilities, to be burned as supplemental fuel in coal-fired boilers and in combustion turbines.
3. Fuel to replace distillate oil and residual oil being burned in boilers and furnaces for space heat in the residential and commercial sectors.
4. Fuel to replace distillate oil for industrial boilers and direct-fired processes.

FUEL FOR MOTOR VEHICLES

Opinions differ on the ease with which the methanol could be introduced as fuel for motor vehicles. Many believe that methanol could be utilized, with adaptation of the engines, in all types of motor vehicles. Also, many believe that a fuel consisting of up to 10 percent methanol in gasoline could be used in gasoline engines with only minor changes in present practices.[3] Even at the 10 percent level, the market would be significant. Further, even if it is determined that the use of methanol pure or at higher concentrations in gasoline, will require time-consuming adjustments, the feasibility of converting methanol to gasoline with the Mobil-M process could open the way for substituting synthetic fuels for unlimited amounts of our gasoline consumption.

Gasoline consumption in 1980 was 2409 x 10^6 bbl (12.66 x 10^{15} Btu).* Ten percent of this total is equivalent to over 60 million tons of methanol. This demand alone would consume the

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*All fuel consumption data taken from Reference 13.

output of eight 25,000-ton/day plants* of the type that has been suggested as an optimum size.[7]

FUEL FOR ELECTRIC UTILITY BOILERS

Utilities currently burn a substantial amount of both distillate oil and residual oil; the distillate is used mostly as a supplemental fuel for startup and for flame stability in coal-fired boilers or in oil-fired combustion turbines. Residual oil is burned as a base fuel in large boilers. Methanol has been demonstrated to be applicable as a substitute for both types of fuel and has been used to fire utility boilers. The 1980 consumption of distillate by electric utilities was 39×10^6 bbl (0.22×10^{15} Btu) and their consumption of residual oil was 438×10^6 bbl (2.75×10^{15} Btu). Replacement of the distillate with methanol would represent a valuable use as a premium fuel and would consume about 10×10^6 tons per year of methanol at present levels of consumption.

Although methanol could be substituted for residual oil as a base fuel, this probably would not be the best application of a premium fuel in light of other possible uses. Substitution for the portion of residual oil that is imported would operate to reduce dependence on foreign oil. But with refineries worldwide necessarily continuing to produce residual oil (as they will for some years), outlets will be needed. Utilities and industrial combustion may be the most effective way to utilize the residual oil, especially that fraction produced in the United States, which is the dominant portion of that used in this country.

FUEL FOR RESIDENTIAL AND COMMERCIAL SPACE HEAT

The residential and commercial sectors consume large amounts of distillate and residual oil, which is used almost exclusively for space heat and could beneficially be replaced by methanol. Substitution for residual oil in these sectors would offer advantages in that the more complex equipment for burning heavy oil in

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*Assumed to be operated at 90 to 95 percent of capacity.

commercial establishments could be eliminated, air pollution reduced, and dependence on foreign oil reduced. Consumption levels in the residential and commercial sectors in 1980 were distillate, 353 x 10^6 bbl (2.06 x 10^{15} Btu), and residual, 86 x 10^6 bbl (0.54 x 10^{15} Btu). This is equivalent to 150 x 10^6 tons of methanol at present levels of consumption.

FUEL FOR INDUSTRIAL BOILERS AND DIRECT-FIRED PROCESSES

Methanol also appears to be a satisfactory substitute for distillate oil in industrial boilers. Distillate oil burned in the industrial sector goes both into boilers and into direct-fired processes such as dryers and kilns. Even though direct-fired processes are highly heterogeneous, it seems reasonable to assume that methanol could be used in almost any situation where distillate is direct-fired. For reasons discussed in connection with utility boilers, the industrial combustion of residual oil is not included as a potential market for methanol fuel, even though it could be used in such applications.

The industrial consumption of distillate oil in 1980 was 257 x 10^6 bbl (1.50 x 10^{15} Btu), the equivalent of 75 x 10^6 tons of methanol.

Table 3 shows a summary of the major applications in which methanol appears to be substitutable.

TABLE 3. SUMMARY OF METHANOL-SUBSTITUTABLE OIL CONSUMPTION (1980)

	Consumption, 10^{15} Btu	Methanol equivalent, 10^6 tons	Oil equivalent, 10^6 bbl
Distillate oil, utility sector	0.22	11	39
Distillate oil, res/comm sectors	2.06	103	353
Residual oil, res/comm sectors	0.54	27	86
Distillate oil, industrial sector	1.50	75	257
Motor gasoline (10%)	1.27	64	241
	5.59	280	976

The total consumption shown in Table 3 amounts to over 15 percent of the total U.S. oil consumption of 34.3×10^{15} Btu in 1980. This figure would be considerably larger if it were assumed that methanol converted to gasoline with the Mobil-M process could be substituted for the entire gasoline consumption of 12.66×10^{15} Btu. Also, amounts for consumption of diesel fuel (2.33×10^{15} Btu in 1979) are not included, even thought it is said to be replaceable with methanol with appropriate engine modifications.

Replacement of the oil products indicated in Table 3 with methanol would require building about thirty-five 25,000-ton/day plants at a cost of about $100 billion. In terms of oil consumption, this comes to a little under 3 million barrels per day, or about 50 percent of our imports. An additional 65 to 70 plants costing around $175 to 200 billion would be required to produce gasoline in amounts equal to 1980 consumption.*

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*Plant sizes assumed and costs estimated are from Reference 7.

PROSPECTS FOR COMMERCIALIZATION OF METHANOL AS FUEL

It is widely accepted that nontechnical problems such as lack of assured markets, unclear policies in regulatory agencies, potential siting difficulties, and related social, economic, and institutional problems are the main barriers to commercialization of methanol fuel or other fuels produced by presently available technologies. Growing pressure for the use of present technology to replace petroleum-derived fuels should alleviate these problems. If it does, the prospects for methanol fuels will depend primarily on advantages they offer over competitive fuels. The following is a discussion of methanol relative to the other fuels that might be produced by present technology to compete, directly or indirectly, with methanol fuels in replacement of petroleum-derived liquid fuels. These are the principal options:

1. Natural gas.
2. Low- or medium-Btu gas made from solid fossil fuels with existing technology.
3. Gasoline derived directly from synthesis gas from coal using Fischer-Tropsch technology.
4. Gasoline produced by subsequent processing of methanol, derived from fossil fuels, using the Mobile-M process.
5. Ethanol produced by fermentation of agricultural crops.
6. Shale oil.

It might be argued that synthetic natural gas (SNG) and fuels produced from direct liquefaction should be considered along with those listed above. They are not, however, because these technologies are not equivalent to the others in terms of stage of development or potential application. Although one SNG plant is reported under construction, this plant will produce supplemental fuel for existing natural gas distribution systems and will not be in direct competition with the fuels being considered. Moreover, the facts do not indicate that direct liquefaction technologies are presently utilizable in the same sense as those used for the above fuels.

METHANOL VERSUS NATURAL GAS

Methanol and natural gas both have potential for replacement of petroleum-derived fuels. Gas can be used directly or as a feedstock for production of methanol. Whether or not natural gas should be used in either way depends on the adequacy of supplies for other critical uses. Until recently the expanded use of natural gas would have been impossible because of short supplies. Since passage of the Natural Gas Policy Act of 1978, which provides for progressive deregulation of natural gas prices, drilling has been increased so that supplies have increased. Although the proven reserves for the lower 48 states were only 195 trillion cubic feed (Tcf) at the end of 1979 (a 10-year supply at 1980 rates of consumption), the total remaining conventional gas resources have been estimated to be 563 to 1219 Tcf.[14] The higher figure is the most recent estimate. In addition, natural gas is known to be recoverable from "unconventional" domestic sources, which include geopressure zones, Western "tight sands", methane from coal seams, and Devonian shales underlying Appalachia.[15,16] Estimates of recoverable natural gas from these resources were recently summarized; these data are presented in Table 4.[16] The wide range of values reflects our present poor understanding of the character of the resources.

TABLE 4. ESTIMATED UNCONVENTIONAL GAS RESOURCES FOR THE UNITED STATES[16]

Resource	Estimated total resource in place, Km^3 (Tcf)	Recoverable resources, Km^3 (Tcf)
Western tight gas sands	1,400-17,000 (49-600)	710-8,860 (25-313)
Eastern devonian gas shales	2,100-20,000 (74-706)	280-14,300 (10-505)
Methane from coal seams	2,000-24,000 (71-847)	450-13,800 (16-487)
Geopressured methane	85,000-1,400,000 (3,000-49,420)	4,200-57,000 (148-2,012)
	90,500-1,461,000 (3,794-51,573)	5,640-93,960 (199-3,317)

In recent months natural gas advocates have argued for "the natural gas option" as a worldwide approach to reducing dependence on oil. They point out that proven worldwide reserves of conventional gas are 2200 Tcf. Estimated remaining undiscovered reserves are said to be 7500 Tcf, giving a total resource that is believed adequate for 50 years even if the present annual worldwide consumption rate of 50 Tcf is doubled.[17] Even if one accepts a lower estimate made in 1975 of 6000 Tcf for total recoverable conventional reserves,[18] the world supplies seem impressive. Utilization of the worldwide gas supplies will, however, require capture of the gas and transport to remote demand points. Some propose that this be accomplished with pipelines and ships transporting liquid natural gas (LNG). Others suggest that where pipelines must be over 5000 miles long or ship transport exceeds 3000 miles, conversion to methanol for shipment is more economical. In addition, the methanol advocates cite the advantages of liquid fuels in markets such as transportation fuels, where natural gas is not widely applicable.[7]

In summary, it appears that natural gas may become increasingly important as a direct substitute for petroleum. At the same time, it also seems appropriate to consider conversion of substantial quantities of natural gas to methanol by present technology to produce direct substitutes for some of the liquid fuels that we are now consuming in amounts equivalent to about 34 x 10^{15} Btu per year. These fuels are now produced partly from domestic oil supplies and partly from about 17 x 10^{15} Btu of imported oil. The magnitude of these numbers is illustrated by comparison with the natural gas consumption for recent years of 20 Tcf/yr, which represents approximately 20 x 10^{15} Btu. No single approach will provide more than a partial solution. Even if the use of natural gas is greatly expanded, there might still be a role for methanol fuels.

METHANOL VERSUS LOW- AND MEDIUM-Btu GAS FROM COAL

Low- and medium-Btu gas can be produced with existing technology and used on-site. Medium-Btu gas, which can be moved by pipeline for short distances, can be produced for use in plants within about 100 miles. Hence, where coal is available near a point of demand, there may be little incentive to produce methanol from coal-derived gas rather than burn the gas directly. Supplies of solid fuel in remote locations, however, might be profitably gasified, converted to methanol, and shipped to distant demand points. This is especially true of low-grade fuels, which are expensive to ship (on a Btu basis) and are more effectively gasified than high-grade coal. Several such plants are being designed to utilize lignite in the United States.[19] Peat, which has little value as fuel except on-site, has also been suggested to be an excellent gasification feedstock. One report indicates that 11,000 and 37,000 square miles of peat bogs with thicknesses of 5 to 25 ft are located in the U.S. and Canada, respectively. The data suggest that the U.S. supply might be equivalent to 6.5 billion tons that could yield about 2.0 billion tons of methanol or 80 x 10^6 ton/yr for 25 years.[20] This annual amount is over 12 percent of our total gasoline consumption in 1980.

METHANOL VERSUS GASOLINE FROM COAL (FISCHER-TROPSCH)

Production of gasoline from coal by the Fischer-Tropsch process might be an attractive alternative for production of non-imported liquid fuels. This technology has been used for many years in South Africa and is being greatly expanded in new capacity. The process, however, produces a wide variety of products for which markets must be available. Further, the quality of the fuel as produced is low relative to methanol fuel or Mobil-M gasoline. Additional processing is required to produce high-octane gasoline. Also, the Fischer-Tropsch process appears to be relatively lower in efficiency and higher in cost, as discussed earlier, when the value of the products is considered. The process does, however, produce a significant amount of gasoline directly, and unless the Mobil-M process is successful, it will be the only currently available option for doing so.

METHANOL FUEL VERSUS GASOLINE FROM METHANOL (Mobil M-Gasoline)

It may be debatable whether the Mobil-M process can be considered available technology, since no full-scale process is in operaton. It is, however, further along in development than other processes in that a commercial plant is to be built. Some consider that processing of methanol in an additional step, as this process does, is unnecessary because methanol is claimed to be usable in amounts of 10 percent or more with gasoline in motor vehicles of conventional design and to be usable pure in motor vehicles of modified designs. Others argue that this is an oversimplification, claiming that certain properties of methanol, including its corrosiveness, toxicity, and affinity for water, constitute problems that would require time-consuming modifications of present practices if methanol is to be widely used in motor vehicles. The Mobil M-Gasoline process in claimed to have 95.5 percent thermal efficiency in conversion, and is said to add only 5¢ per gallon to the cost of output fuel.[21] If this performance is attainable, the technology could be quite useful in attaining faster penetration for coal-derived fuels in the transportation fuel market.

METHANOL VERSUS ETHANOL FROM FERMENTATION OF CROPS

Ethanol from fermentation of crops is being used as motor fuel both in the United States and abroad. Problems and advantages associated with its use are in many ways similar to those associated with the use of methanol. Ethanol is, however, subject to certain unique limitations, primarily associated with availability of raw materials. Thus, even though ethanol production is a useful technology, it may be more limited in applicability than that for methanol fuels, in the long run.

Ethanol plants are expected to be relatively small so that they can be located near raw material supplies (such as corn) and near outlets for byproduct animal feed, the sale of which is essential to process economics. Also they effectively remove land from food production at a time when there is already concern over the rate at which farm land is being lost to other uses. Experience to date suggests that ethanol will play a role in replacement of petroleum fuels but is not likely to be a dominant contributor.

METHANOL VERSUS FUEL FROM OIL SHALE

Fuels from shale oil, like M-Gasoline, have not been produced commercially, but plans have been made for commercial plants. There is a considerable body of pilot plant data to support the scaleup of oil shale processes. The technical risk for commercial plants appears to be minimal. Further, oil shale deposits are very extensive and could supply our oil needs for hundreds of years. Because of economic uncertainties, however, developers are reluctant to make firm committments without such incentives as guaranteed markets. Hence, prospects are poor for near-term production of large amounts of synfuel from oil shale. Also, crude feedstocks from oil shale are of low quality compared with methanol. Thus, it appears that markets for methanol fuel should exist even if shale oil ventures are highly successful.

CONCLUSIONS

Methanol fuel technology appears to be very cost-competitive with other technologies that could be applied in a synthetic fuels industry today. Although the projected cost of methanol fuels is somewhat higher than today's prices for distillate oil and gasoline, methanol fuel plants built now could prove to be highly profitable at prices that may prevail when they come on stream.

The "clean burning" characteristics of methanol make it potentially attractive from the standpoint of combustion system design and control of environmental impacts associated with its use. Also, methanol is easily transportable and could be produced from abundant supplies of low-grade fossil fuels located in regions of the United States remote from points of demand for premium fuels. Hence, technology for production of methanol could be applied to utilize energy supplies that would otherwise be of limited usefulness.

Methanol fuels seem to be an attractive alternative to premium fuels in several critical applications that are expected to grow in importance. One of the most important involves replacement of gas and distillate oil fired in turbines used by utilities for peaking, in combined cycles, or "repowering" to increase the capacity of existing power plants.

The use of methanol fuel technology to convert natural gas to liquid fuels as a short-term solution for oil shortages should be given serious consideration. Markets in which methanol fuels could be substituted are large and represent a significant portion of our current oil imports. The amounts of natural gas that could be produced over the next 20 years are highly controversial. The optimistic estimates suggest that allocation of significant quantities to production of liquid fuels could be helpful in solution of short-term problems.

A thorough study of possibilities for the use of methanol fuels on a wide scale is needed. Such a study should begin with analysis of gaps in the available information, which has been developed in piecemeal studies conducted over the past 10 to 15 years. This full-scale analysis should lead to definitive conclusions with respect to the policies to be adopted in future energy programs.

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CONVERSION AND EQUIVALENCY FACTORS

1 bbl (barrel) = 42 gallons

1 bbl gasoline = 5.4×10^6 Btu

1 bbl methanol = 2.7×10^6 Btu

1 ton methanol = 20×10^6 Btu

1 ton methanol = 7.4 bbl methanol and is equivalent to 3.7 bbl gasoline

1 Tcf (trillion cubic feet) of natural gas = 10^{15} Btu

1 Km^3 (cubic kilometer) of natural gas = 35.3×10^9 cf (cubic feet)

1 Km^3 of natural gas = 35.3×10^{12} Btu

Density of gasoline = 5.8 lb/gal

Density of methanol = 6.6 lb/gal

A 25,000 ton/day methanol plant produces 8.2×10^6 ton/yr which is equivalent to 30.3×10^6 bbl of gasoline.

Motor gasoline consumption for the U.S. was $2{,}409 \times 10^6$ bbl in 1980. This is equivalent to 12.66×10^{15} Btu. This amounts to 6.3×10^6 bbl/day.

Oil imports for 1980 were 6.8×10^6 bbl/day. This included refined petroleum products amounting to 1.6×10^6 bbl/day (3.2×10^{15} Btu/yr) and crude oil amounting to 5.2×10^6 bbl/day (10.4×10^{15} Btu/yr).

Natural gas consumption in the United States in 1980 was 21.5 Tcf, which is equivalent to 21.5×10^{15} Btu or 10.7×10^6 bbl/day of crude oil.

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METHANOL AS AN ALTERNATIVE TRANSPORTATION FUEL†

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ABSTRACT

Over the remaining years of this century synthetic fuels will play a key role in the nation's drive for energy independence. Although self-reliance is indeed a desirable goal, many people believe it cannot be achieved without significant compromises in environmental quality. This may not be the case. One synfuel, methanol, could be used to replace both gasoline and diesel fuel and yield environmental benefits. This paper compares methanol with synthetic fuels from other coal liquefaction processes in terms of the environmental and economic consequences of their use.

INTRODUCTION

Several factors must be addressed when considering the viability of an alternative motor fuel. These can broadly be grouped into two categories, environmental and economic. Each of these categories would include the production, distribution, and in-use aspects of the fuel in question. In the report that follows, we have attempted to address these issues for several alternative automotive fuels, especially methanol, which could be produced from coal. In addition to methanol from indirect liquefaction, fuels from the following technologies were examined: the Mobil Methanol to Gasoline (MTG) indirect liquefaction process, and the Exxon Donor Solvent (EDS), H-Coal, and Solvent Refined Coal (SRC-II) direct liquefaction processes.

Of the subjects examined below, the environmental analyses of production and distribution are the most general since the least amount of information was available in these areas. Although more detail is provided in other sections, the preliminary nature of the entire report should be emphasized. More work is needed before final conclusions can be stated with confidence.

ENVIRONMENTAL

PRODUCTION AND DISTRIBUTION

It should first be recognized that coal itself contains many diverse elements and compounds in addition to hydrogen and carbon, such as organic nitro-compounds, organic and inorganic sulfur, and trace metals, such as lead, arsenic, etc. The conversion of coal to other fuels offers a number of opportunities for these pollutants to reach the environment in harmful ways, regardless of the particular conversion process used.

One potential advantage of processes which gasify coal, such as those leading to methanol or gasoline (via methanol), is that the gasification itself places most of the potentially harmful elements and compounds into forms which can be removed relatively easily. For example, minerals and heavy metals are removed from the gasifier as slag which cools to a solid. While the high concentration of metals, etc. requires careful disposal, this disposal may not be as difficult as that connected with coal liquefaction. With direct coal liquefaction, these compounds are entrained in the heavy organic liquid and must be separated from the liquid phase later in the process. This solid-liquid separation is very difficult (basic research is still underway in this area[1]) and the separation from a solid cannot be made as completely as the separation from a gas. Inevitably, some liquid will end up with the solid waste and some heavy metals will be left in the crude fuels. Thus, not only may the solid waste disposal problem be worsened by the addition of complex, polycyclic organic material to the waste, but the fuel itself still contains more minerals and heavy metals.

One factor which may mitigate or eliminate this problem for most direct liquefaction processes is the high probability that most of the heaviest liquid fraction will be gasified to produce hydrogen.[2,3] If this is done, most of the minerals and heavy metals can be removed from the gas fairly early, since this heavy liquid fraction should contain most of the coal's impurities. Thus, the full extent of this disadvantage may depend primarily on the fraction of the impurities which can be removed via gasification and the fraction which must be removed directly from the liquid itself.

Another potential advantage of gasification over direct liquefaction is the fact that all of the organic nitrogen and sulfur is broken down to simple compounds like ammonia and hydrogen sulfide. These are relatively easy to separate from the carbon monoxide and hydrogen which make up the major part of the synthesis gas. Also, since the carbon monoxide and hydrogen must be essentially free of nitrogen and sulfur before reacting over the catalyst to form methanol, there is an economic incentive to remove these two elements. Although the nitrogen which is not removed prior to the catalyst will be removed by the catalyst itself, slowly deactivating it, any unremoved sulfur would rapidly deactivate the catalyst.

Coal liquefaction, on the other hand, inherently leaves most of the sulfur and nitrogen in the liquid phase, bound with the organics. The most effective technique to remove these compounds is hydrogenation, which also is used to upgrade the fuel. However, hydrogenation is expensive, because of the large amounts of hydrogen consumed, and will likely be limited to only the degree that is necessary to market the fuel.[4] If the fuel is upgraded to gasoline or high quality No. 2 fuel oil, most of the sulfur and nitrogen will be removed and there should not be any significant problems. However, that portion of the synthetic crude which may be burned with little or no refinement could contain relatively high levels of these elements and represents more of an environmental hazard than gasification products.

The remaining distinct difference between the environmental effects of coal gasification and coal liquefaction processes (prior to end-use) is in exposure to the fuel itself, after production and in distribution. While coal liquids are for the most part hydrocarbons and, as such, are similar to petroleum, they are more aromatic and contain significant quantities of polycyclic and heterocyclic organic compounds. Some of these compounds are definitely mutagenic in bioassays and many have produced tumors in animals. Thus, while the noncarcinogenic health effects of these materials would be more similar to those of crude petroleum, they would definitely have the potential to be more carcinogenic. There is also some evidence that much of this bioactivity can be removed by moderate to severe levels of hydrogenation which would occur if high grade products were produced. Thus, again the potental hazard is dependent upon the degree of hydrogenation given the products.

Indirect liquefaction products, on the other hand, do not appear to exhibit mutagenicity or carcinogenicity. Methanol is neither mutagenic nor carcinogenic and early tests run on M-gasoline have shown it to be nonmutagenic, similar to petroleum-derived gasoline. Therefore, either of these two products offers some degree of benefit over direct liquefaction products. It is possible, however, that methanol produced from coal may contain impurities and that such impurities may affect exhaust products when used. Research needs to be done in this area, also.

Methanol, of course, is highly toxic in heavy exposures, leading to blindness or death. Much of its notoriety in this area is due to people confusing it with ethanol and drinking it in large quantities. Hydrocarbon fuels, while also toxic, do not suffer from this confusion and are not often taken internally. With proper education of the public, confusion between methanol and ethanol should be minimized. However, more work is still needed in this area also.

The final point which deserves mention here is the difference between the effect of an oil spill and a methanol spill. The effects of oil spills are well known; oil films stretching for miles, ruined beaches, surface fires, etc. The effects of a methanol spill are expected to be quite different, primarily because methanol is soluble in water. While high levels of methanol are toxic to fish and fauna, a methanol spill would quickly disperse to nontoxic concentrations and, particularly in water, leave little trace of its presence afterward.[5] Sea life should be able to migrate back quickly and plant life should begin to grow back quickly, though complete renewal would take the time necessary for new plants to grow back. Also, if a methanol fire does start, it can be effectively dispersed with water, which is not possible with an oil fire. However, methanol flames can be invisible, making them more difficult to avoid.

The various relative environmental aspects of synthetic fuels production and use mentioned above are those which appear to stand out at this time. More work, however, is still needed in most areas. Although natural gas to methanol plants exist and have led to much experience in handling methanol, questions related to methanol production from coal are not known with absolute certainty since such large scale facilities do not currently exist. Similarly, no real life experience of the effects of the production of synthetic crudes exists, nor of their use. Given these caveats and the need for further research, however, the indirect liquefaction route to yield methanol or gasoline (from methanol) appears to have some potential environmental advantages over direct liquefaction processes.

VEHICLE USE

The data presented below were obtained from tests of actual methanol engines. However, it should be noted that these data were taken using engines which were only roughly converted to use of methanol; fully optimized engines would be expected to show further improvements in fuel efficiency and emissions.

The worst problem concerning methanol's actual use centers around its low vapor pressure and high heat of vaporization. These properties make it difficult to start a neat methanol engine in cold weather.[6] Also, methanol has a very low cetane number of approximately 3, which means that it is very difficult to ignite in a compression-ignition engine (e.g., a diesel). Problems associated with materials compatibility and lubrication also exist, but these problems already appear to be solvable with existing technology, requiring only that the auto designer know that methanol is going to be the engine fuel.

Various techniques are already being tested which will improve the cold-starting capability of gasoline engines operating on methanol, such as better mechanical fuel atomization, electrical fuel preheating, and the blending of volatile, low boiling point components into the methanol. Methanol's ignition problems are more serious in diesel engines, but several possible solutions are being investigated, such as glow plugs and spark ignition. Brazil already has an experimental methanol-fueled diesel running on the road which uses relatively inexpensive glow plugs as ignition aids and M.A.N. in Germany has designed a diesel bus engine with spark ignition which runs on methanol.[7,7a]

As will be seen later in the section on fuel consumption in the economics section, the fuel properties of methanol which lead to these difficulties also lead to many advantages, such as increased thermal efficiency relative to gasoline engines. Past experience with both gasoline and diesel engines has shown that the disadvantages of a fuel can usually be overcome to allow exploitation of the advantages, particularly when the advantages are as large as they appear to be for methanol.

Methanol engines promise improved emission characteristics over gasoline and diesel engines in a number of areas. Especially important are low emissions of nitrogen oxides (NOx) and an absence of emissions of particulate matter, heavy organics and sulfur-bearing compounds. One possible side benefit of methanol use could be that precious metal catalysts might not be needed for emissions control. Because methanol fuel will contain no sulfur, phosphorus, lead, or other metals, base metal catalysts (e.g., nickel, copper, etc.) may suffice. One likely negative impact of methanol engines would be an increase in engine-out aldehyde emissions, particularly formaldehyde. Catalytic converters, however, would be expected to reduce aldehyde emissions to acceptable levels. The available data supporting these effects are discussed below.

A search of the literature shows a general consensus that methanol engines produce approximately one-half of the NOx emissions of gasoline engines at similar operating conditions, with individual studies showing reductions between 30 percent and 65 percent.[8,9,10,11,12] One of the major engine design changes expected with methanol engines is the use of higher compression ratios to increase engine efficiency. Experiments have confirmed the theoretical expectation that these higher compression ratios, with no other design changes, will increase NOx emissions considerably due to the higher combustion temperatures.[13,14] However, with high compression ratios, less spark timing advance is needed. Retarding spark timing is known to reduce both NOx emissions and engine efficiency. Fortunately, it has been shown that the combination of a much larger compression ratio with a few degrees of spark timing retard can both increase thermal efficiency and decrease NOx emissions.[14] This raises the possibility of methanol vehicles being able to meet the current 1.0 gram per mile NOx emission standard without the need for a NOx reduction catalyst.

Use of methanol in a diesel engine should also reduce NOx emissions by the same degree as that described above. Diesel engines have higher peak combustion temperatures and the effect of a cooler-burning fuel should actually be even more apparent in a diesel than in a gasoline engine. Unfortunately, no data to confirm this is yet available from a diesel engine running on pure methanol. However, emission tests have been performed on a dual-fuel diesel, where a small amount of diesel fuel is injected to initiate combustion of the methanol. These tests have shown NOx emission reductions as high as 50 percent.[15,16]

These lower NOx emissions would aid many areas of the country in attaining the ambient standard for NO_2 in the future. (Most areas are currently under compliance with the NO_2 ambient air quality standard, but many are projected to exceed it in the future as NOx emissions continue to rise.) Lower NOx emissions would also help alleviate the acid rain problem, though the majority of this problem appears to be due to stationary source emissions. Finally, the use of methanol would also provide a method for heavy-duty engines to reduce NOx emissions closer to the congressionally-mandated level without giving up any of the fuel economy advantage of diesels, as will be seen later.

The lack of hard data on diesels operating on pure methanol indicated above will also be evident below as other aspects of methanol-fueled diesel engines are discussed. The basic reason for this lack of data is that until recently methanol has not been seriously considered to be an acceptable fuel for a diesel engine because of its very low cetane number. For many years, studies examining methanol as an engine fuel concentrated on gasoline-type engines (fuel inducted with combustion air). However, as the more recent studies are indicating, it appears possible to burn methanol in a diesel accompanied with some kind of ignition assist and, therefore, utilize the efficiency of the diesel concept.

In addition to the positive effect on NOx emissions, use of methanol engines should provide even greater benefits with respect to emissions of particulate matter and heavy organics from diesels. Gasoline engines operated on unleaded fuel emit only small quantities of particulate matter, composed primarily of sulfate particles. Thus, any improvement in particulate emissions from switching to methanol from gasoline would be small.

However, diesel engines emit large quantities of particulate matter consisting of solid carbonaceous particles (soot) and liquid aerosols. The former are generally formed when the injected fuel droplets are incompletely combusted, leaving carbon particles. These solid particles can then serve as nuclei for more harmful organic species to adsorb onto and as "vehicles" for such compounds to reach (and possibly lodge in) the deep regions of the lung. Although reductions in diesel engine particulate have been reported, particulate matter seems to be an inherent pollutant in diesel-fueled compression ignition engines.

Methanol, on the other hand, is a "light" fuel relative to diesel fuel and should produce far less carbonaceous particles, as do other hydrocarbon fuels "lighter" than diesel fuel. In addition, since methanol does not contain inorganic materials like sulfur or lead, there should not be any other types of solid particulate formed. Accordingly, with pure methanol there would be no nuclei for liquid aerosols to adsorb onto and total particulate emissions would be expected to be near zero. [17] This is certain to be the case with a well designed methanol-fueled spark-ignition engine. [18] Unfortunately, however, we know of no studies which have measured particulate from compression ignition engines burning neat methanol. Several studies (all of which used a small amount of diesel pilot fuel) have reported much lower smoke levels, both in single-cylinder tests and in a 6-cyclinder, turbocharged, direct-injected engine. [7,15,19] There seems to be little question, however, that neat methanol combustion in compression ignition engines would result in very low (and possibly zero) particulate emissions. This would result in a very important environmental advantage compared to diesel fuel combustion.

As mentioned earlier, formaldehyde emissions from methanol engines are of some concern since there is some evidence that formaldehyde is carcinogenic. Formaldehyde is an intermediate specie in methanol oxidation and would be expeced to be emitted from methanol engines in greater quantities than either diesel or gasoline engines. Many studies have shown total aldehyde emissions (mostly formaldehyde) from methanol engines to be two to ten times greater than aldehyde emissions from gasoline engines. [20,21,22,23]

At the same time, catalytic converters have been shown to be effective in removing approximately 90 percent of exhaust aldehydes. [9,10,23,24] Much research has been performed regarding the parameters which influence aldehyde formation in gasoline engines, with low exhaust temperatures and high oxygen concentrations identified as leading to higher formaldehyde formation rates, and this knowledge should facilitate aldehyde control in future engine designs. [22,25] Aldehyde emissions from methanol combustion in diesel engines are also expected to be greater than from diesel fuel combustion.

The last benefit of methanol engines to be discussed concerns sulfur emissions. Because of the way methanol is produced it contains essentially no sulfur. And, if there is no sulfur in the fuel, no emissions of sulfur-bearing compounds, such as sulfur dioxide, sulfuric acid, or hydrogen sulfide, can occur. This is a slight improvement over gasoline emissions, since gasoline does have a small amount of sulfur in it. Catalyst-equipped gasoline engines currently emit between 0.005 and 0.03 grams per mile of sulfate and this would disappear with the use of methanol, even if catalysts were still used.

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The improvement over the diesel, however, would be more pronounced. Diesel fuel currently contains 0.2-0.5 percent sulfur by weight. This translates into about 0.25 grams per mile of elemental sulfur from diesel trucks (0.5 grams per mile of sulfur dioxide, or 0.75 grams per mile of sulfate, equivalent). Diesel cars emit about one-fifth this amount. Since the sulfur level in diesel fuel is expected to rise in the future, these emission levels would also rise in the future. With the use of methanol these emissions would disappear altogether.

ENVIRONMENTAL SUMMARY

Although coal contains many substances which could be environmentally damaging, it appears that indirect liquefaction processes, methanol and Mobil MTG, can facilitate their removal easier than is possible through direct liquefaction routes such as EDS, SRC-II and H-Coal. Further, since indirect liquefaction necessitates the removal of all sulfur before the fuel is synthesized, the use of relatively cheap base metal catalysts (as opposed to noble metals currently in use) on automobiles is a possibility.

Neither methanol nor Mobil M-gasoline appear to exhibit mutagenicity or carcinogenicity. It should be remembered, however, that commercial coal-to-methanol plants are not yet available so the influence of possible impurities is not yet known. Direct coal liquefaction products are more aromatic and contain significant quantities of polycyclic and heterocyclic organic compounds, some of which are mutagenic. There is some evidence, however, that much of this bioactivity can be removed by moderate to severe levels of hydrogenation. More work needs to be done in these areas before definitive conclusions can be reached.

The effects of a methanol spill are expected to be quite different from that of the classical oil spill since methanol is soluble in water. Although high levels of methanol are toxic to fish, a methanol spill should quickly disperse to nontoxic levels.

Methanol engines promise emission benefits over both gasoline and diesel engines. Lower emissions of nitrogen oxides, and the virtual absence of particulate matter, heavy organics and sulfur bearing compounds from vehicle exhaust are promising. A possible detriment of methanol engines is that they emit higher amounts of aldehydes, principally formaldehyde which is carcinogenic. Catalytic converters, however, have been shown to be effective in removing 90 percent of exhaust aldehydes. As was the case with the environmental consequences of synfuel production, more work needs to be done in the vehicle-use area as well.

ECONOMIC

We have analyzed a large number of studies in order to estimate the costs associated with the production and use of synthetic fuels. A superficial review of their conclusions quickly revealed a wide variety of conclusions and recommendations. One reason for this is that the economic bases used by the various studies often differ, affecting costs by as much as 100 percent. Another reason is that each study uses the best information available at the time of the study. Since the product mixes, efficiencies and costs of many of these processes, especially the direct liquefaction processes, change frequently as more is understood about the process, studies performed even 2 or 3 years ago cannot be compared to the latest studies.

Thus, we have attempted to go back in each instance to the original engineering studies to assess the viability of the cost estimates. We also have compared the available designs of each process to ascertain which are out-dated or based on now inaccurate assumptions. After doing this, the projects were placed on the same economic basis and adjusted for plant size.

While the difficulties and apparent discrepancies described above primarily involve the costs of producing synthetic fuels, the overall economic picture involves more. The entire process of producing synthetic fuels and using them in motor vehicles will be broken down into three areas. The first area consists of the production of a usable liquid fuel from raw materials. The second area consists of distribution of this fuel. Finally, the third area includes the use of these fuels in motor vehicles. All costs will be presented in 1981 dollars. It should be noted that the general approach followed in this section is from a long-term perspective. That is, we have not identified any detailed costs associated with the implementation of methanol as a "new" transportation fuel.

PRODUCTION COSTS

Determining the economics of the production of usable synthetic liquid fuels is probably the most difficult of the three areas to be examined. The engineering and financial bases that have been chosen are shown in Tables 1 and 2. As shown in Table 1, two different sets of financial parameters were chosen. These were selected from a survey of recent studies[26,27,28,29, 30,31] done on coal liquefaction processes and represent two extreme cases for capital charge. The low capital charge rate and accompanying parameters were chosen from the ESCOE report[26] while the high capital charge data were taken from the Chevron study.[28] The important factors yielding these two CCRs are also shown in Table 1.

Table 2 shows the remaining input factors. All plants were normalized to 50,000 fuel oil equivalent barrels per calendar day

TABLE 1. COMMON FINANCIAL PARAMETERS

Financial Parameters	Low Cost Case[26]	High Cost Case[28]
Capital Charge Rate, Percent	11.5	30
Debt/Equity Ratio	40/60	0/100
Discounted Cash Flow Rate of Return on Investment, Percent	Not Available	15
Project Life, Yrs.	20	20
Construction Period, Yrs.	4	4
Investment Schedule, %/Yr.	9/25/36/30	10/15/25/50
Plant Start Up Ratios	50, 90, 100...	50/100
Debt Interest, Nominal Rate, Percent	10	-
Investment Tax Credit, %	9	10
Depreciation Method	Sum of Year's Digits	Sum of Year's Digits
Tax Life, Yrs.	15	13

TABLE 2. PROCESS COST INPUTS AND OTHER FACTORS COMMON TO ALL STUDIES

Cost Inputs and Other Factors	Value
Product Yield	50,000 FOEB/CD
Coal	
a) Bituminous	$27.50/ton
b) Subbituminous	$17.00/ton
c) Lignite	$10.00/ton
Operating Costs	
a) Utilities	$0.035/kw-HR
b) Working Capital Interest	6% of working capital per year.
c) Fuel Cost	$35/bbl
Scaling Factors	
a) Capital Costs	0.75
b) Labor Costs	0.20
c) Maintenance, Taxes, Insurance, General	Same percentage of plant investment as specified by each individual study.
d) Coal, Catalysts and Chemicals, Utilities, Fuel, Natural Gas	Amount varies directly proportional to plant size.
By-Product Credit	
a) Sulfur	$50/ton
b) Ammonia	$180/ton
c) Phenol	$112.6/bbl
Contingency factor	15%
Inflation Rate	
a) 1976	5%
b) 1977	6%
c) 1978	7%
d) 1979	9%
e) 1980	9%
Real Cost Increases (%/year)	
a) Fuel Oil	2%
b) Natural Gas	2%
c) Coal	0%

(FOEB/CD)(one FOB equals 5.9 mBtu, higher heating value). The costs selected for bituminous, subbituminous and lignite coals are respectively $27.50, $17.00, and $10.00 per ton. Because capital costs do not usually vary in direct proportion to plant size, a scaling factor (an exponent) is normally used to modify the ratio of plant sizes (by yield). The scaling factor used here was 0.75, which is an average of factors found from various studies.[29,31, 32,33] To adjust labor and supervision costs a scaling factor of 0.2 was used.[26,32] The rest of the operating costs were assumed to vary directly with plant size. The inflation rate for adjusting the costs of studies to $1981 was based on the Chemical Engineering plant cost index.

The product mix expected from each of the various synfuel processes being investigated can be found in Table 3. In order to put the discussion on costs into a more meaningful perspective, several points should be kept in mind. First, indirect liquefaction processes can yield a product mix which is either essentially 100 percent transportation fuel or a 50-50 mix of transportation fuel and SNG. The latter appears to be more efficient and economical for either methanol or MTG-gasoline production, but the cost of producing essentially 100 percent transportation fuel will be used here since the nation's energy shortfalls are primarily in the transportation area. Second, the product mix from direct liquefaction processes depends largely on the degree of refining applied. Each of the direct liquefaction procedures yields some SNG or LPG which can be sold without further processing, while the remainder of the products in most cases must be refined before marketing. This refining adds to the product's cost. Third, the mixes reported in Table 3 were taken from available refining reports. The SRC-II study was based on maximizing gasoline production while the EDS and H-Coal studies also considered No. 2 fuel oil production. Fourth, none of the synfuel processes being examined produce residual oil or diesel fuel. Residual oil could of course be obtained by the direct liquefaction routes simply by applying less refining. However, products from direct liquefaction plants appear to be too high in aromatics to allow economical production of diesel fuel.

Turning once again to Table 3, it can be seen that capital costs range from $2.04 billion to $3.3 billion. The methanol plants tend to have the lowest capital costs ($2.0-2.5 billion), while that of the EDS process is in the same range near the high end. Using the incremental cost of the MTG process, a gasoline-from-coal plant would cost between $2.6 billion and $3.1 billion. The H-Coal and SRC-II processes are next at $3.3 billion. (The capital costs do not include refinery costs since it is unlikely that new refineries would be built.)

A product value approach was utilized to estimate costs for individual products. This technique assumes that the future prices of particular fuels will maintain a certain relationship, based on relative demand. All prices are normalized relative to a reference pro-

TABLE 3. PRODUCT AND CAPITAL COSTS OF SELECTED COAL LIQUEFACTION PROCESSES (1981 DOLLARS)

Process	Product Mix	Refined Product Cost ($/mBtu)		Capital Cost* (Billions of Dollars)
		11.5% CCR	30% CCR	
Direct Liquefaction				
EDS (Bituminous)	32.7% Reg. Gasoline	10.11	16.57	2.50
	14.0% Prem. Gasoline	10.87	17.81	
	25.6% No. 2 Fuel Oil	8.29	13.59	
	9.6% LPG	7.78	12.76	
	18.1% SNG	8.09	13.26	
H-Coal (Bituminous)	50.7% Reg. Gasoline	8.41	16.13	3.30
	11.0% Prem. Gasoline	9.04	17.34	
	20.1% No. 2 Fuel Oil	6.90	13.23	
	18.2% LPG	6.48	12.42	
SRC-II (Bituminous)	64.7% Gasoline	9.87	19.06	3.30
	12.1% LPG	7.60	14.68	
	23.2% SNG	7.90	15.24	
Indirect Liquefaction				
Texaco (Bituminous)	100% MeOH**	5.90-6.16	9.80-10.00	2.06
Koppers (Bitum.)	100% MeOH**	6.97	11.73	2.51
Lurgi (Subbit.)	47.9% MeOH**	5.82	10.02	2.32
	49.7% SNG	6.03	10.55	
	2.4% Gasoline	7.54	13.19	
Modified Winkler (Lignite)	100% MeOH**	5.25	9.12	2.04
Lurgi Mobil MTG (Subbit.)	41.2% Reg. Gasoline	7.54	13.19	2.92
	53.3% SNG	6.03	10.55	
	5.5% LPG	5.80	10.16	
Mobil MTG Incremental Cost	85-90% Reg. Gasoline 10-15% LPG	1.72	3.17	0.6

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* Capital costs are instantaneous costs. Capital costs do not include refinery capital costs.

** MeOH = 95-98% methanol, 1-3% water, and the remainder higher alcohols.

duct, which here was chosen to be gasoline. In this report, a relationship between various fuels similar to that reported in the ICF report was used and is as follows:

1. If the cost of unleaded regular gasoline is \$G/mBtu,
2. The cost of No. 2 fuel oil is (0.82)(G)/mBtu, and
3. The cost of LPG is (0.77)(G)/mBtu.[29]

Since unleaded premium gasoline is produced in some cases (EDS and H-Coal), a relationship between this fuel and regular gasoline is also necessary. Unfortunately, a history of the relationship between these two fuels was not readily available. The cost ratio of leaded premium to leaded regular gasoline was used instead. This relationship indicated a cost ratio of 1.075.[34] This product cost relationship was then applied to premium and regular unleaded gasoline.

The cost for SNG was assumed to be (0.8)(G). This value was obtained by averaging those for No. 2 fuel oil and LPG since SNG should share markets with each, especially No. 2 fuel oil.

The product costs, along with capital costs discussed earlier, are shown in Table 3. As can be seen, they follow a similar pattern as capital costs, though not exactly. Speaking first of the low cost scenario, methanol is the cheapest product, ranging from \$5.25-\$6.97 per million Btu (mBtu) for fully commercial gasifiers and \$5.90-\$6.16 per mBtu for the near commercial Texaco gasifier. Gasoline via the Mobil MTG process would be \$1.72 per mBtu more, or \$6.97-\$7.69 per mBtu using fully commercial gasifiers and \$7.62-\$7.84 per mBtu with the Texaco gasifier. H-Coal gasoline costs slightly more at \$8.41 per mBtu, while SRC-II gasoline is projected to cost \$9.87 per mBtu. Finally, EDS gasoline is projected to cost the most of the automotive products at \$10.11 per mBtu.

A similar order holds for the higher cost scenario. In this case, SRC-II has replaced EDS as the process yielding the highest cost product. This is primarily due to the higher capital costs involved for SRC-II. It should also be noted that the absolute difference between methanol costs and the cost of gasoline from the other processes increases because the capital cost of the methanol plant is lower. The same is true for MTG gasoline in most cases. A large change occurs in the difference between EDS and H-Coal process costs. While the EDS costs were 20 percent higher using the low CCR, they are less than 3 percent higher using the high CCR.

Using all the studies which are publicly available, it would generally appear that the indirect coal liquefaction processes can produce usable fuel cheaper than the direct liquefaction technologies.

DISTRIBUTION COSTS

Since distribution systems already exist for gasoline, the economics in this area would, of course, favor the continued use of this fuel over the introduction of methanol. In addition, gasoline also has the advantage of possessing a higher energy density: 115,400 Btu/gal for gasoline compared with 56,560 Btu/gal for methanol. Thus, because transportation costs depend primarily on volume, gasoline would necessarily be less expensive to transport per Btu.

The costs of distributing a fuel can most easily be divided into three areas; 1) distribution from refinery or plantgate (if no refining is required) to the regional distributor, 2) distribution from the regional distributor to the retailer, and 3) distribution by the retailer (i.e., the gas station). These three aspects of distribution will be discussed below.

More detail could of course be added to this analysis to improve the resulting estimates but such information has not yet been assimilated. However, the general conclusions reached below should not change substantially.

To simplify the presentation here, long-range distribution is approximated by that of pipeline transport to a distance of roughly 650 miles.[29] It should be noted that if pipelines are needed to connect coal fields (where synfuel plants are likely to be located) with major markets, then the total costs will be roughly the same whether the plant produces methanol or synthetic gasoline. This is evident since the pipeline must be built in either case and the construction and operating costs increase only slightly with a doubling in size. Further, right-of-way and engineering costs should not change at all with capacity in this range.

In the case of distributing methanol, the total amount of energy distributed would only be about 80 percent that of gasoline due to vehicle efficiency improvements which will be discussed later. However, a gallon of methanol only contains half the energy contained in a gallon of gasoline, so 60 percent more volume of methanol would need to be transported than that of gasoline.

To determine the potential range of the cost of transporting methanol, two bracketing assumptions can be made. One, the cost of transport per volume of fuel can be assumed to remain constant. Two, total distribution costs can be assumed to remain constant. With the first assumption, the estimated cost for gasoline transportation is $0.22 per mBtu.[29] Methanol transportation would cost twice this amount or $0.44 per mBtu. Using the second assumption, where total costs remain constant, the cost for methanol would be $0.27 per mBtu, since only 80 percent as much energy is being transported. Thus, the cost of long-range distribution of methanol is $0.27-0.44 per mBtu.

The costs involved with a switch to methanol will be more related to the increase in volumetric capacity than differences in chemical properties. Pipelines and pumps are almost entirely made from steel or brass, with which methanol is compatible. Rubber seals on pumps may need to be replaced with more durable rubber compounds, but this should be a minor cost.

As mentioned earlier, the next step of local distribution consists of storing fuel at the regional distributor and transporting it to the retailers. This distribution is primarily done by tanker truck and is estimated to cost just over $0.05 per gallon of gasoline, or $0.46 per mBtu. If one conservatively assumes that the cost per volume remains constant, the $0.46 per mBtu cost for gasoline would translate into a $0.92 per mBtu cost for methanol.

Here the cost of conversion to methanol should be very small, even negligible. The only change required should be new rubber seals and hoses, if they were not already made from a material compatible with methanol.

The costs of retailing fuel (the last step) are more like that of long-range distribution than local distribution. The costs of retailing are primarily fixed costs, such as land or rent. Retailing differs from both long-range and local distribution, however, in that fuel energy is the critical marketing factor, not volume.

Typical retailer mark-ups are estimated to be in the range of $0.05-0.18 per gallon of gasoline.[35] However, since the lower mark-ups are usually associated with the high-volume stations, the average mark-up per gallon of gasoline sold in the U.S. should be somewhere between $0.09-0.11, or $0.76-0.95 per mBtu. For methanol, the cost would lie between this range and 25 percent more since the total amount of energy distributed would be 20 percent less. Thus, the cost of retailing methanol would be $0.76-1.19 per mBtu.

In deriving these retail costs, no attempt was made to account for any additional costs the retailer would bear when methanol is first introduced. For example, he will have to make some monetary allowance for the initial small volume of customers. The retailers in some instances will also incur costs associated with installing new tanks if the existing ones are incompatible or unavailable due to large demands for the specific fuels they contain. The abovementioned retailing costs should therefore be considered as long-term costs, after the methanol market stabilizes.

The total cost of distributing methanol and gasoline can now be calculated by simply combining the costs presented in the last three sections. Methanol would cost $1.95-2.55 per mBtu to distribute; gasoline would cost $1.44-1.63 per mBtu. Gasoline has a significant advantage over methanol in terms of percentage (26-36 percent lower), but the absolute difference is only $0.51-0.92 per mBtu.

IN-USE COSTS

In order to determine in-use costs associated with methanol, it is necessary to know its fuel efficiency characteristics. There is general agreement among researchers that methanol is a more energy efficient vehicle fuel than gasoline. There are at least two theoretical reasons why this is so. One, methanol's lower flame temperature reduces the amount of heat transfer from the combustion chamber to the vehicle coolant system. Two, its high heat of vaporization acts as an internal coolant and reduces the mixture temperature during the compression stroke. These characteristics are realized in experiments without having to make any major design changes in current gasoline engines. Studies have shown these inherent properties of methanol to increase the energy efficiency of a passenger vehicle by 3 to 10 percent with a middle range of about 5 percent.[9,12,13]

Other properties of neat methanol combustion allow even greater efficiency improvements. Its wider flammability limits and higher flame speeds relative to gasoline allow methanol to be combusted at leaner conditions while still providing good engine performance. This lean burning capability decreases the peak flame temperature even further and allows more complete combustion, improving energy efficiency. Early testing on a single-cylinder engine yielded estimated energy efficiency improvements of 10 percent due to leaning of the methanol mixture as compared to gasoline tests.[36] Subsequent vehicle testing has shown relative efficiency improvements of lean methanol combustion of 6 to 14 percent.[8,9] Given these results, it would appear that methanol's lean burning capability yields approximately a 10 percent efficiency improvement over and above the 3-10 percent improvement mentioned above. Of course, stratified charge engines have been developed to allow leaner combustion of gasoline as well, and this efficiency advantage of methanol would be lessened with respect to a stratified charge engine.

Methanol's higher octane number also allows the usage of higher compression ratios with correspondingly higher thermal efficiencies. Early single-cylinder testing have estimated the thermal energy efficiency improvements of the higher compression ratios to be in the range of 16 to 20 percent.[14,36] Unfortunately, little vehicle data exist to confirm these figures, but it must be expected that improvements of at least 10 to 15 percent are likely.

Adding up the possible improvements indicates that methanol engines may well be 25 to 30 percent more energy efficient than their gasoline counterparts when the methanol engine is designed specifically for methanol.

However, since such methanol engines are not available for mass distribution today, this section will use a more conservative fuel efficiency advantage for methanol engines over their gasoline counterparts of 20 percent. Using a fuel economy of 30 miles per gallon for the average gasoline-fueled vehicle, this average vehicle would require about 0.0038 mBtu per mile to operate. A methanol-fueled vehicle would be expected to use at least 20 percent less energy or about 0.0030 mBtu per mile.

Using 12,000 miles per year and the average delivered fuel costs, calculated by combining production and distribution costs, the annual fuel savings relative to gasoline produced via indirect liquefaction (Mobil MTG process) were determined (see Table 4). These savings include two separate effects. One, they include the effect of differences in at-the-pump fuel costs. Two, they also include the effect of methanol engines being more fuel efficient than gasoline engines. For consistency, all fuels were assumed to be derived from bituminous coal.

Following this procedure and using the lowest fuel cost (based on the low CCR) and the highest fuel cost (based on a 30 percent CCR), methanol would produce a savings of $131-240 per year compared to gasoline from the Mobil MTG process. Direct liquefaction gasoline would cost an extra $36-410 per year over MTG gasoline, because of its potentially higher at-the-pump cost.

To this fuel savings must be added any difference in engine or vehicle cost. While a methanol-fueled diesel engine may be developed with a fuel efficiency advantage comparable to that of a standard diesel, the conservative 20 percent efficiency advantage over the gasoline engine should be attainable with engines similar to the gasoline engine in terms of both design and cost. While a larger fuel tank and a special cold start system may increase costs, savings should be attained with respect to emission control, particularly if NOx reduction catalysts are no longer needed and if base metal oxidation catalysts can be used instead of platinum and paladium. Thus, whether a methanol engine will cost more or less than a gasoline engine in the long run is still an open question at this time. It would be rather safe to project, however, that any potential extra cost would not override the kind of fuel efficiency benefit described earlier.

ECONOMICS SUMMARY

The results of the past three sections are shown in Table 4. As can be seen when the results are combined, methanol compares favorably to the other fuels. With respect to synthetic gasoline, methanol appears to cost less at the plant gate. This is true whether the low CCR is used or the high CCR. Higher distribution costs lower the difference, but even after distribution, methanol appears to still hold some advantage. This advantage is $1.21- $2.25 per mBtu over MTG gasoline and $2.00-$6.41 per mBtu over direct liquefaction gasoline. For vehicles driven 12,000 miles per year and achieving 30 miles per

TABLE 4. SYNTHETIC FUEL COSTS ($ per mBtu)*

	Indirect Coal Liquefaction		Direct Coal Liquefaction
	Methanol	Gasoline	Gasoline
Production			
Plantgate Cost	5.90-11.73	7.62-14.90	8.41-19.06
Distribution			
Long-Range	0.27-0.44	0.22	0.22
Local	0.92	0.46	0.46
Retail	0.76-1.19	0.76-0.95	0.76-0.95
Cost at Pump	7.85-14.28	9.06-16.53	9.85-20.69
ANNUAL FUEL SAVINGS (RELATIVE TO GASOLINE AT $9.06-16.53 per MBtu)**			
	$131-240	$0	$-(36-189)
ADDED ENGINE COST OVER GASOLINE ENGINE			
	0	0	0

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* Range of plantgate cost is the lowest cost using the low CCR and the highest cost using the high CCR for bituminous feedstocks.

** Includes effect of increased engine efficiences and differences in at-the-pump fuel costs.

gallon (gasoline), methanol would save \$131-\$240 per year over MTG gasoline and \$167-\$429 per year over direct liquefaction gasoline if allowances are made for the increased efficiency of methanol engines. Without including the improved engine efficiency, annual savings would be \$55-\$103 relative to MTG gasoline and \$91-292 over direct liquefaction gasoline.

It should be stated that no comparison was made between methanol and diesel fuel since none of the coal conversion processes examined produces diesel fuel of sufficient quality for today's diesel engines. All of these economic results are of course subject to the qualifications which have been stated previously; the primary ones being that the detail of the engineering designs could not be compared across processes, and that cost estimates reflect different points of development for different synfuels.

CONCLUDING STATEMENT

Looking back over the topics addressed in this paper, it can be concluded that at this point in time methanol appears to have environmental and economic advantages over other synthetic transportation fuels derived from coal. The ultimate viability of this conclusion depends on a number of key events or findings. One, a cost-competitive methanol engine must be able to meet the driveability needs of most of the U.S. (e.g., cold-starting in nearly all climates). Two, aldehyde emissions must be controllable at low cost. Three, no other unique and uncontrollable environmental problems of methanol use or production are discovered. Four, the production and distribution cost comparisons made here must hold up against future scrutiny.

The probability of these events occurring can only be estimated by a review of the support for each presented in this study. At this time, we believe the evidence available suggests that the benefits of methanol outweigh its costs.

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PROJECT SUMMARY

A COMPENDIUM OF SYNFUEL END USE TESTING PROGRAMS†

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ABSTRACT

A "Compendium of Synfuel End Use Testing Programs", which provides information on major recently-completed, current and planned synfuel end use testing projects, has been developed. The compendium is intended to promote flow of information among various synfuel testing programs, thereby reducing chances for duplication of effort and enabling design and implementation of cost-effective and systematic approaches to the collection of appropriate environmental data in conjunction with ongoing and planned performance testing projects. It is EPA's intention to update this compendium to include results from current and future testing programs.

Projects described in the compendium involve testing of shale-derived fuels, SRC-II middle distillates, EDS fuel oils, H-coal liquids and methanol-indolene mixtures in various equipment such as utility boilers, steam generators, diesel engines (lab-scale and full-scale), auto engines, and various other combustors. Published reports on various testing efforts and discussions with test sponsors/contractors are the sources of data for the compendium.

Based on the data presented in this compendium, the thrust of the synfuel testing program which has been carried out to date has been to assess equipment performance and fuel handling characteristics. Where some emissions monitoring has been conducted, such efforts have been limited in scope and have primarily emphasized measurement of criteria pollutants (NO_x, SO_x, particulates, etc.). Essentially no data have been collected on emissions of non-criteria/non-regulated pollutants.

INTRODUCTION AND OBJECTIVES OF THE COMPENDIUM

A recently-completed synfuel utilization background study* identified a great need for better coordination among various agencies involved in synfuel

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*M. Ghassemi and R. Iyer, "Environmental Aspects of Synfuel Utilization", EPA Report No. EPA-600/7-81-025, March 1981. (Note: For a summary of this report, see Environmental Science and Technology, Volume 15, No. 8, August 1981, pp. 866-873.)

end use testing programs so as to promote more systematic approaches to the collection of environmental data in connection with such programs and to reduce chances for duplication of effort. Per recommendation of the background study, a compendium of synfuel end use testing programs has been developed as an information source on major recently completed, ongoing, and planned synfuel end use testing programs. The dissemination of the document among agencies/organizations engaged in various aspects of synfuel production, testing, utilization, and regulation, coupled with holding regular symposia/workshops on synfuel utilization and end use testing, should greatly enhance coordination and flow of information among various programs and, in the long run, contribute to the goal of more rapid establishment of an environmentally acceptable commercial synfuel industry in the U.S. EPA plans to periodically update this compendium to include results from current and future testing programs.

DATA BASE USED AND DATA PRESENTATION

Information presented on the synfuel testing programs has been obtained from published documents and via telephone calls and/or interviews with organizations involved in the testing programs. The key individuals/agencies providing most of the reports and data used in the compendium are listed in Table 1.

A separate "data sheet" has been devoted to each project covered in this compendium to permit periodic updating of the document to include additional projects and incorporation of further results from ongoing studies. The data sheets are grouped into four categories, covering projects for which the key sponsors/participants are Electric Power Research Institute (EPRI), Department of Defense (DOD), Department of Energy (DOE), and Miscellaneous agencies (e.g., EPA). Data sheets are presented for a total of 44 projects, of which 7 are in the EPRI-sponsored category, 15 in the DOD category, 13 in the DOE category, and 9 in the Miscellaneous category.

Where data have been available, each data sheet provides the following information on a test project: type of fuel tested (both synfuel and the reference petrofuel, where indicated), test equipment used, test site, test objectives, sponsoring agency, contractor, test conditions, environmental monitoring, project status, summary of results, and references (where a report or reports have been published on a project).

A summary of the data contained in the data sheets is presented in Table 2. Tables 3 and 4 present brief descriptions of some of the recently initiated and tentatively planned synfuel testing programs. Two examples of the data sheets are presented.

OVERVIEW OF SYNFUEL TESTING PROGRAMS

Based on the data presented in the test program data sheets and summarized in Table 2, and on the discussions which have been held with a number of synfuel developers, trade associations and potential major users of synfuels,

TABLE 1. LIST OF ORGANIZATIONS/INDIVIDUALS PROVIDING INFORMATION USED IN THE DEVELOPMENT OF THE COMPENDIUM

Electric Power Research Institute
3412 Hillview Drive
Palo Alto, CA 94303
Mr. Al Dolbec

Air Force Wright Aeronautical
Laboratory, Aero Propulsion Laboratory
Wright-Patterson AFB/POSF
Dayton, Ohio 45433
Mr. Charles Delaney

Navy Air Propulsion Center
P. O. Box 7176
Trenton, NJ 08628
Mr. C. J. Nowack

David W. Taylor Naval Ship R&D Center
Code 2705
Annapolis, MD 21402
Mr. Carl A. Hershner

Army Mobility Equipment Research and
Command Center - Attn: DRDME-GL
Ft. Belvoir, VA 22060
Mr. F. Schaekel

U.S. Air Force HQ AFESC/RDV
Tyndall AFB
Tyndall, FL 32403
Major J. Tom Slankas

DOE, Bartlesville Energy
Technology Center
P. O. Box 1398
Bartlesville, OK 74003
Mr. Dan Gurney

DOE, Conservation and Solar Energy Div.
Washington, D.C.
Mr. Gene Ecklund

DOE, Office of Coal Utilization
Fossil Energy Research Center
Germantown, MD
Mr. John Fairbanks

DOE, Laramie Energy Technology Center
P. O. Box 3395
Laramie, WY 82071
Dr. R. Poulson

DOE, Pittsburgh Energy Technology
Center, Analytical Chemistry Division
Pittsburgh, CA
Mr. Curt White

National Aeronautics and Space
Administration, Lewis Research Center
21000 Brook Park Drive
Cleveland, OH 44135
Mr. Rick Niedzwiecki

EPA, Special Studies Branch
Industrial Environmental Research Lab.
Research Triangle Park, N.C. 27711
Mr. G. Blair Martin

EPA, Motor Vehicle Emission Laboratory
2625 Plymouth Road
Ann Arbor, MI
Mr. Robert Garbe

EPA, Combustion Research Branch
Industrial Environmental Research Lab.
Research Triangle Park, N.C. 27711
Mr. G. Blair Martin

EPA, Office of Environmental
Engineering and Technology
Industrial Environmental Research Lab.
Research Triangle Park, N.C. 27711
Mr. W. S. Lanier

EPA, Mobile Sources Laboratory
Research Triangle Park, N.C.
Mr. Frank Black

Southwest Research Institute
Automotive Research Division
6220 Culebra Road
San Antonio, TX 78284
Mr. Charles T. Hare

Southwest Research Institute
Mobile Energy Division
6220 Culebra Road
San Antonio, TX 78284
Mr. John A. Russell

U.S. Department of Transportation
Systems Center
Kendall Square
Cambridge, MA 02142
Mr. Joe Sturm

U.S. Department of Energy and
Coordinating Research Council
Atlanta, GA
Mr. Al Zingle

Carson Associates for
Bank of America
4117 Robertson Boulevard
Alexandria, VA 22309
Mr. Gavin McGurdy

Energy and Environmental Research
Corporation
8001 Irvine Boulevard
Santa Ana, CA 92705
Mr. Dave Pershing

Ford Motor Company
Scientific Research Laboratory
Dearborn, MI

Vulcan Cincinnati, Inc.
Cincinnati, OH
Mr. R. W. Duhl

TABLE 2. SYNFUELS-COMBUSTION SYSTEM COMBINATIONS TESTED AND EMISSIONS MONITORED

Test No.	Agency	Synfuel	Reference Fuel	Combustion System	Emissions Monitored	General Conclusions
1	EPRI	SRC-II fuel oil	No. 6 fuel oil	Tangentially-fired utility boiler	NO_x, CO, THC, SO_3, POM, particulates, particle size, particulate composition	• No adverse boiler performance effects with SRC-II fuel. • NO_x emissions nominally 70% higher than No. 6 fuel.
2	EPRI	SRC-II fuel oil H-Coal EDS oil	No. 6 and No. 2 fuel oils	Scaled-down utility boiler	NO, CO_2, CO, SO_2, SO_3, THC, smoke, particulates, particle size	• Higher fuel nitrogen content of SRC-II fuels produced higher NO emissions than reference fuels. • NO emissions from H-Coal and EDS liquids were lower than SRC-II. • No unique differences in combustion or emission characteristics of SRC-II fuel blends.
3	EPRI	SRC-II fuel oil	No. 2 and No. 5 fuel oil	Babcock & Wilcox package boiler	NO_x, CO, CO_2, SO_2, hydrocarbons, O_2, and dust	• NO_x emissions consistent with fuel nitrogen content. • Combustion performance of SRC-II fuel oil was similar to No. 2 and No. 5 fuel oils.
4	EPRI	SRC-II, H-Coal	No. 2 diesel fuel	Three catalytic reactors	NO_x and CO	• Coal-derived liquids can be burned catatytically but SRC-II, and to a lesser degree H-Coal, appeared to degrade reactor performance significantly as evidenced by higher CO emissions. • NO_x emissions were consistent with fuel nitrogen content.
5	EPRI	Hydrogenated shale oil and various liquid fuels for SRC-I, H-Coal, EDS, and SRC-II	No. 2 distillate fuel	Full-scale and sub-scale turbine combustors	NO_x, CO, UHC, particulates, and smoke	• A selected number of coal liquids and shale oil fuels can be used in current turbines. • Emission levels of CO, UHC, and particulates for synfuels were about the same as for No. 2 fuel - not significant. • Significant quantities of FBN are converted to NO_x causing emissions higher than EPA limits.
6	EPRI	Solvent refined coal	Bituminous coal	Utility boiler	NO_x, SO_2, CO_2, particulates, particulate composition	• The boiler stayed much cleaner with SRC than with coal, producing an equivalent boiler efficiency as coal at full load. • The quantity of SRC flyash was 10 to 15% of that of coal flyash with no bottom ash accumulation from SRC. • Particulates, SO_2 and NO_x emissions from SRC were all under EPA limits.
7	EPRI	*	Jet-A fuel, natural gas, methanol	Two utility gas turbines	NO_x, CO, SO_2, THC, POM, sulfates, particulates, aldehydes, opacity	• Methanol is a suitable fuel for gas turbines; turbine performance and NO_x and particulate emissions are improved over the other fuels.

(Continued)

TABLE 2. (Continued)

Test No.	Agency	Synfuel	Reference Fuel	Combustion System	Emissions Monitored	General Conclusions
8	DOD	Shale-derived JP-5 and blends with petroleum JP-5	Petroleum JP-5	DOD helicopter engine: Allison T63-A-5A turboshaft	NO_x, CO, CO_2, and THC	• NO_x emissions increased with increasing fuel nitrogen content; conversion efficiency was about 45%. • No significant effects were noted on engine performance or CO, CO_2, and THC emissions due to the presence of high levels of fuel bound nitrogen.
9	DOD	Shale-derived DFM	Petroleum diesel fuel (MIL-F-16884G)	U.S. Navy LM2500 turbine engine	NO_x, CO, THC, and smoke	• Combustor and engine operating characteristics were identical when using marine diesel or DFM shale oil; thus, DFM shale oil would be suitable for use in LM2500 engines. • NO_x emissions followed fuel nitrogen content; CO and THC levels were essentially the same for both fuels.
10	DOD	JP-5 from oil shale, coal, and tar sands	Jet-A, JP-5, diesel marine fuel, leaded gasoline, and blends of the above	Two high temperature/pressure research combustors	NO_x, CO, UHC, and smoke	• In all performance areas, the synfuels correlated in the same manner as petroleum-derived fuels except for NO_x emissions from the shale oil fuel. • Smoke formation was dependent on hydrogen content; combustion efficiency, CO, and UHC depend more on higher boiling point components than fuel viscosity.
11	DOD	Shale fuel oil	Petroleum diesel fuel marine (DFM)	Steam generator diesel engine	Particulates and particulate composition	• No significant differences between particulate emission products measured in the study from the combustion of DFM or shale fuel oil.
12	DOD	Shale-derived diesel fuel	Petroleum distillate	Lab-scale diesel engine	NO_x, THC, and smoke	• There was no significant difference in performance or emissions with the shale-derived fuel.
13-15	DOD	Shale-derived DFM	Petroleum DFM	3 different types of prototype steam generators	NO_x, SO_2, CO, CO_2, THC, O_2, and smoke	• There were no significant differences in measured pollutant emissions resulting from the combustion of petroleum DFM or shale-derived DFM on the CVA-60, DDG-15, and the FF-1040 boilers. In each case, SO_2, NO_x, and smoke were below levels set by EPA.
16	DOD	Oil shale-derived JP-5 fuel	Petroleum-derived JP-5 fuel	DOD helicopter engine: Allison T62-A-5A turboshaft	NO_x, CO, and THC	• Performance, CO, and THC emissions were equivalent for both fuels. • NO_x emissions followed fuel nitrogen content.

(Continued)

TABLE 2. (Continued)

Test No.	Agency	Synfuel	Reference Fuel	Combustion System	Emissions Monitored	General Conclusions
17	DOD	Unifined kerosene derived from tar sands	Petroleum-derived JP-5 fuel	DOD helicopter engine: Allison T63-A-5A turboshaft	NO_x, CO, and UHC	• Unifined Kerosene was a satisfactory substitute for petroleum JP-5 fuel. • NO_x emissions were slightly higher when using unifined kerosene than with JP-5.
18	DOD	Distillate, aviation, turbine, and diesel fuels derived from coal, tar sands and oil shale	Various petroleum-derived fuels	Wide variety of Army power-plant systems	Various pollutants	• Product quality of many synfuels tested and other results are described in individual abstracts.
19-21	DOD	*	13 petroleum derived fuels: JP-4, JP-8, diesel No. 2 & various blends	General Electric F101 turbofan, J79-17C turbojet, and J79 turbojet engines	NO_x, CO, UHC, and smoke.	• In all three engines, fuel hydrogen content strongly affected smoke and NO_x emissions. NO_x emissions were also highly dependent upon combustor operating conditions.
22	DOD	*	12 petroleum-derived fuels: JP-4, JP-8, and various blends	TF41 turbofan combustor	NO_x, CO, UHC, and smoke	• All pollutant emissions measured were highly dependent upon operating conditions. CO and smoke levels were also strongly affected by hydrogen and aromatic content of fuels.
23	DOE	SRC-II middle distillate	Low quality residual oil, and petroleum reference distillate fuel	Combustor sized for use with industrial gas turbine	NO_x, CO, CO_2, THC, and smoke	• The combustor was able to achieve low NO_x with all fuels. • CO and smoke varied directly with rich zone equivalence ratio and inversely with lean zone equivalence ratio.
24	DOE	SRC-II middle distillate	Petroleum distillate	Various combustor concepts	NO_x, smoke	• Values of NO_x were reduced for the smaller diameter quench zone and increased for larger diameter quench zone. • Rich-lean burn stage combustion system can meet EPA emission standards.
25	DOE	SRC-II middle distillate	Low quality residual oil and distillate fuel	Seven combustors of varying designs for use in utility gas turbine engines	NO_x, smoke, CO, unburned HC	• A lean-lean combustor has potential for achieving ultra-low NO_x emissions with distillate, residual or other fuels containing up to 0.25% (wt.) fuel nitrogen. CO and smoke met program goals from this combustor also.
26	DOE	SRC-II middle distillate	Low quality residual oil, petroleum reference distillate oil, and natural gas	Combustors for use in utility gas turbine engines	NO_x, CO, THC, smoke	• Lean-lean combustor NO_x emission levels were higher than emission goals using SRC-II fuel. CO emissions remained low using SRC-II fuel, while no smoke was detectable and UHC levels were negligible throughout these tests. • Rich-lean combustor NO_x emissions appeared to reach a minimum below the NO_x emission goal for rich primary zone condition.

(Continued)

TABLE 2. (Continued)

Test No.	Agency	Synfuel	Reference Fuel	Combustion System	Emissions Monitored	General Conclusions
27	DOE	SRC-II middle distillate	Low quality residual oil, petroleum reference distillate oil	Experimental combustor for use with utility gas turbine engines	NO_x, CO, UHC, smoke	• Five combustors have been found adequate for further development: rich-lean diffusion flame venturi quench, burner ceramic lined pipe lean burner, multiannular swirl burner, Rolls-Royce combustor, and lean catalytic combustor. These meet NO_x emission limits set by EPA with petroleum distillate and/or residual oils. • SRC-II fuel NO_x emissions were close to meeting EPA limits in only two combustors: rich-lean diffusion and ceramic lined pipe lean burners.
28	DOE	SRC-II middle and heavy distillate, fuel oils & three blends of the above	No. 2 and No. 6 petroleum-based fuel oils	A 20-hp Johnston, fire-tube boiler	NO_x, SO_2, CO, HC and polynuclear aromatic hydrocarbons	• The levels of NO_x and SO_2 produced were proportional to the amount of nitrogen and sulfur in the fuel. • There appear to be two sources of trace organics in the exhaust gases: small amounts of the fuel itself not burned during combustion, and the products of combustion. For the petroleum fuels, n-alkanes and polynuclear aromatic hydrocarbons are seen in the exhaust gas; for the SRC-II fuels, the alkanes are absent or present at very low levels, and polynuclear aromatic hydrocarbons not seen in the petroleum exhaust gases are present.
29	DOE	*	Indolene and 10% methanol/90% indolene	Two light duty vehicles	Evaporative emissions (hydrocarbons and methanol)	• Using methanol 10% blend increased evaporative emissions by 130% for short term use and 220% for long term use.
30	DOE	*	Unleaded gasoline and methanol/indolene mixtures	Auto engines (10)	NO_x, CO, THC, aldehydes, and methanol	• Aldehyde, methanol, and hydrocarbon emissions increased with higher concentration of methanol in the fuel. • CO was reduced by the addition of methanol to the base fuel.
31	DOE	*	10% methanol/90% gasoline blends	Auto engines (7)	NO_x, CO, and evaporative emissions (HC and methanol)	• Data show consistent reduction in CO emissions with use of methanol blends. • Significant increases in evaporative emissions with methanol blends.
32-34	DOE	*	Ethanol, methanol, and gasoline blends	Fleet vehicles	Evaporative and tailpipe hydrocarbon emissions	• 75% increase in evaporative emissions with methanol blends over a straight gasoline. • Emissions were lower for vehicles fueled with gasohol but data was inadequate to conclude a significant difference.
35	DOE	*	Indolene, indolene/methanol blends and ethanol/indolene blends	Pontiac 4-cylinder modified engine	Total aldehydes and specific organics	• Total aldehydes increased 25% in going from indolene to ethanol/indolene and methanol/indolene blends. • Formaldehyde is the largest component of the total aldehydes (up to 90 mole percent of the total).
36	Vulcan Cincinnati	*	No. 6 residual oil, natural gas, and methanol	Small scale boiler test stand and a 49 MW utility boiler	NO_x, CO, and aldehydes	• In the utility boiler, methanol NO_x levels were 7-14% of those measured during residual oil combustion. • CO emission levels of methanol were less than 100 ppm and generally less than those observed for the residual oil. • Aldehyde emissions during methanol combustion were generally less than 1 ppm.
37	Ford Motor Co.	*	Methanol, indonele, and blends	Ford 400 CID engine and 1975 Ford LTD with 400 CID engine	Total hydrocarbons and specific organics	• Methanol/indolene blends gave significantly higher hydrocarbon and aromatic emissions than indolene without a catalyst, but only slightly higher emissions with a catalyst.

(Continued)

TABLE 2. (Continued)

Test No.	Agency	Synfuel	Reference Fuel	Combustion System	Emissions Monitored	General Conclusions
38	DOT	Shale-derived DFM	No. 2 diesel fuel	VW Rabbit engine	NO_x, CO, THC, particulates, Ames test on particulates	• HC and CO emissions were found to be lower and NO_x levels higher for the shale-derived fuel as compared to the petroleum-derived fuel. Particulate emissions were similar for both fuels. • Mutagenic activity of the organics from the particulate matter was similar for the two fuels.
39	Bank of America	*	Methanol/gasoline blends	Fleet vehicles	NO, CO, unburned hydrocarbons	• Blends of 2 to 18% methanol decrease emissions of CO and unburned hydrocarbons and result in improved mileage in new cars. • Certain blends result in operating cost decreases of 1¢/mile.
40	EPA	Shale-derived DFM	No. 2 fuel, and No. 2 fuel with 0.5% nitrogen	Two configurations of a full-scale prototype (25-MW engine-size) gas turbine combustor utilizing a Rich burn/Quick Quench combustor concept	NO_x, CO, unburned hydrocarbons	• Both combustor configurations met program emissions goals using both reference fuels and synfuel. • Unburned HC emissions from one combustor ranged from 0.9 to 7.3 ppmv for No. 2 fuel; 1.1 to 21.8 ppm for No. 2 fuel with 0.5% nitrogen; and 1.3 to 15.3 ppmv for shale-derived DFM at 15% O_2.
41	EPA	SRC-II middle distillate fuel oil and shale-derived residual oil	No. 2 fuel oil and Indonesian/Malaysian residual oil	Prototype full-scale (25-MW engine-size) Rich Burn/Quick Quench gas turbine with two combustor configurations	NO_x, CO, unburned hydrocarbon, and smoke	• All emissions exhaust goals met. • Relationship demonstrated between primary zone residence time and attainable NO_x emission concentrations.
42	EPA	*	Residual and distillate oils, natural gas, propane, isopropanol, methanol	Experimental wall furnace and prototype industrial boiler	NO_x, NO, CO, HC, and aldehydes.	• NO emission levels for the five fuels were as follows: distillate oil > propane > isopropanol > alcohol mixture > methanol. • Although there was considerable scatter in the data, aldehyde concentrations were around 10 ppm for methanol. • NO emissions for all fuels decreased with increasing fraction of flue gas recirculation. • CO and hydrocarbon emissions were always below 50 ppm and smoke was not observed for any fuel.
43	EPA	*	No. 5 residual oil, natural gas, and methanol	Industrial water-tube and fire-tube boilers	NO_x	• Flue gas recirculation was capable of reducing NO_x emissions during methanol combustion. • Methanol NO_x emissions were significantly lower than during residual oil combustion and were also less than during natural gas combustion.
44	EPA	*	Indolene and ethanol blends	Two light duty vehicles	NO_x, CO, THC, ethanol, and evaporative emissions	• The addition of ethanol to indolene reduced tailpipe emissions of THC and CO, but increased NO_x. • Use of gasohol increased evaporative emissions substantially.

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*Because of the unavailability of synfuels, the fuels used in some of these programs were not "true" synfuels (e.g., methanol-derived from natural gas was used instead of coal-derived methanol). These studies, however, are included in this report because they were conducted to show what might be expected from the combustion of actual synfuels in the indicated combustion systems.

TABLE 3. ON-GOING SYNFUEL TESTING PROGRAMS

Sponsoring Agency	Test Fuels	Time Period	Project Description
EPA, Motor Vehicle Emission Laboratory	Shale-derived diesel fuel and SRC-II fuel versus National Average Baseline Diesel Fuel.	1981 to ---	Volkswagen Rabbit diesel engine testing. Emissions monitored to include particulates, NO_x, CO/CO_2, hydrocarbons, and aldehydes.
	Mobil-M gasoline.	1981	Oldsmobile 350 and other engines testing. Emissions monitored include particulates, NO_x, CO/CO_2, and hydrocarbons.
DOE, Bartlesville Energy Technology Center; Contractor/test site:			
A. General Electric, Erie, PA	SRC-II middle distillate and oil shale distillate	1981	Testing of GE EDI-8, 8-cylinder "V" configuration, 5344 cu. in. standing diesel engine for electric power, rail and marine applications. Parameters being evaluated include: starting ability, injection timing, fuel rate variation effects and internal engine temperatures. Emissions monitored include O_2, CO/CO_2, NO_x, SO_2, HC, H_2SO_4 and particulates.
B. Transamerica Delaval, Oakland, CA	SRC-II middle distillate	1981	Testing of Delaval DSR 46, 6-cylinder in-line configuration, 28,600 cu. in. standing diesel engine for electric power, compressor and marine applications. Performance parameters being evaluated include starting ability, precombustion chamber effects, ignition delay, and other engine parameters. To date, the engine has been operated at full load using a pre-mixed blend of 60% SRC-II liquid and 40% diesel oil which had been injected into the combustion chamber with no modification of the engine, followed by increasing proportions of SRC-II liquid up to 100%. Emissions monitored include O_2, CO/CO_2, NO_x, SO_x, THC, and smoke.
C. A.D. Little Beloit, WI	SRC-II middle distillate	1981	Fairbank-Morse 38 to 8-1/8, 6-cylinder opposed piston design, 3108 cu. in. standing diesel engine for electric power and marine applications, compressors and pumps being tested. Parameters being evaluated include effects of load variations, combustion pressure vs. time, and engine delay. Emissions monitored include CO/CO_2, NO, NO_2, SO_2, SO_4, HC, PAH, particulates and oxidants.
D. Energy and Environmental Research Springfield, OH	Shale-derived distillate oil and Exxon Donor Solvent coal-derived liquids	1981	Testing of Superior 6-cylinder in line configuration turbo-charged 4120 cu. in. standing diesel engine for use in compressors, pumping and electrical power generation. The purpose of the tests is to compare engine performance parameters during synfuel and conventional fuel combustion. Tests with shale-derived distillate oil and a baseline No. 2 diesel fuel include SASS train sampling for PAH and particulate. Other emissions monitored include CO, HC, NO_x, and smoke. Tests with Exxon Donor Solvent liquids will probably include the above procedures and also pilot injection and pre-injection starting tests.

(Continued)

TABLE 3. (Continued)

Sponsoring Agency	Test Fuels	Time Period	Project Description
E. Acurex Shoreham-by-the-Sea, England	Shale oil residuals.	1981	Testing of A.P.E. Allen BSC 1/8 6-cylinder, in-line configuration, 5101 cu. in. standing diesel engine for marine, pumping, compressor and electric power applications. Tests include injection, starting, combustion duration and steadiness. Emissions monitored include CO/CO_2, NO_x, NO_2, THC, and smoke.
DOE, Conservation and Solar Energy Division	Various shale- and coal-derived fuels.	1978-1981	Auto engine dynamometer testing being conducted at SwRI. Particulates, NO_x, CO/CO_2, hydrocarbons, and aldehydes being monitored.
	SRC-II distillates and shale-derived JP-5 and DFM mixed with powdered carbon, sawdust, or other cellulosic material.	1981 to ---	Slurry/fuel project involving diesel engine testing. Particulates, NO_x, and other emissions being monitored.
	Coal-derived methanol and gasohol.	1981 to ---	Testing in 1,000 fleet vehicles; program currently constrained for lack of fuel samples.
DOE, Office of Coal Utilization	SRC-II and shale-derived fuels.	1980 to ---	Medium speed diesel engine testing conducted by SIMI-Pielstich, Paris; Baumester Wain, Copenhagen; Grandi Motori Trieste, Trieste; and Selzer of Switzerland.
	SRC-II middle distillates, a 2.9 to 1 blend of SRC-II middle and heavy distillate, and shale-derived fuels.	1980 to ---	Program conducted at Norwegian Technical Institute in various ships.
	SRC-II middle distillate.	1981 to ---	Continuation of low NO_x fuel combustor concept program (see TTM 32-36). Several combustors to be tested by Westinghouse; staged combustor to be tested at several operating loads at Detroit Diesel Allison; testing of 5 combustors planned at GE.
DOE, Pittsburgh Energy Technology Center	Biomass fuel, H-Coal, Exxon Donor Solvent, and shale fuel oils.	1981 to October 1982	Continuation of small scale combustion of synthetic fuels program (see Test 28). A 20-hp firetube boiler is to be tested with the above synfuels using No. 2 and No. 6 fuel oils as a baseline. The purpose of the program is to assess the possible environmental impact of substituting synfuels for petroleum in utility and industrial boilers.
Department of Transportation and Rutgers University	Coal- and shale-derived diesel fuel.	1981 to 1982	Testing of a recently-designed and constructed one cylinder diesel engine, including collection of particulates and other combustion products.
Sandia Laboratories	Petroleum-derived synfuel simulation fuels, with higher hydrocarbon/aromatic content than conventional fuels.	1981 to ---	Testing being conducted in single cylinder diesel systems and auto/truck engines from Cummins Engine Co. Emphasis on measurement of flame fronts and other engine/burn parameters. Limited emissions monitoring performed.
Bank of America	Methanol/gasoline blends.	1980 to ---	Testing being conducted in blends ranging from 2 to 18% methanol in fleet vehicles, with emphasis on blends of 2 and 4%. CO, NO, and unburned hydrocarbons being monitored.

TABLE 4. TENTATIVE SYNFUEL TESTING PROGRAMS

Sponsoring Agency	Fuels to be Tested	Time Period	Project Description
Army, MERADCOM, Ft. Belvoir, VA	Diesel fuels and other synfuels (high aromatic content fuels, low lubricity fuels).	1982 to ---	Development of accelerated fuel qualification test procedures, including matrix of specific Army equipment components and candidate fuels; project is part of Army Alternative Fuels Program.
Air Force/Navy/EPA (Under the direction of Capt. H. Cewell, USAF Civil Engineering and Services Center, Tindall AFB)	Shale-derived JP-4, JP-5, and JP-8.	Late 1981	Collection of particulates from various engine combustion tests for toxicity and biological effects testing.
Navy Air Propulsion Test Center (NAVSSES), Trenton, NJ	Various shale-derived fuels.	Pending receipt of synfuel samples	Testing of synfuels in various test burners and aviation equipment.
AF Wright Aeronautical Lab, Aero Propulsion Laboratory, Wright-Patterson AFB, Cincinnati	Various shale-derived fuels.	1982-1983	Engine augmenter tests and whole engine tests on 3 engines; emissions monitoring for NO_x, CO/CO_2, and hydrocarbons.
EPRI	Various liquid and solid synfuels, including shale-derived heavy and middle residuals, and methanol	1981-1986	Testing of synfuels in various diesel engines, turbines, and boilers; limited emissions monitoring for SO_x, NO_x, CO/CO_2, O_2 and/or particulates.
EPA, Motor Vehicle Emission Laboratory	EDS and H-coal liquids	Late 1981 to September 1982	Large standing diesel engines and a GE research engine, using same contractors as on-going programs (see Table 3). Particulate matter to be collected.
	SRC-II fuel	1982	Electronically controlled internal combustion engine at UTC, East Hartford, CT. Limited emissions monitoring.
EPA, Industrial Environmental Research Laboratory, RTP, N.C.	Coal-derived middle and heavy distillates; shale-derived No. 2 fuel oil, methanol (technical grade); and petroleum reference fuels	1981-1982 (Phase I)	Comparative synfuel/petrofuel combustion testing in a 2.5 MM Btu/hr packaged boiler and in a 165 kw stationary diesel to identify conditions leading to major differences in emissions, and to develop recommendations for comparative testing.

the following are some general observations on the status, nature, and thrust of the synfuel testing programs:

- Since the primary use of synfuel products is expected to be as combustion fuels, nearly all synfuel end use testing programs have involved evaluation of fuel suitability for use in combustion systems (auto engines, industrial/utility boilers, turbines, etc.).

- Reflecting the developmental status of the synfuel technologies, the thrust of the synfuel testing programs which have been carried out to date has been to assess equipment performance and fuel handling characteristics. Where some emissions monitoring has been conducted, such monitoring efforts have been limited in scope and have primarily emphasized measurements of gross parameters such as particulates, NO_x, SO_x, etc., emissions. The limited scope of the monitoring programs has also been in part due to: (a) an absence of a clear definition of the specific environmental data which would be required on synfuel products by regulatory agencies (e.g., by EPA's Office of Pesticides and Toxic Substances in connection with the Premanufacturing Notification Section of the Toxic Substances Control Act); and (b) lack of a standard protocol for testing for environmental data acquisition.

- Most of the synfuel end use testing programs have been, or are being, conducted/funded by DOD, EPRI, and DOE. The programs of these organizations have, respectively, emphasized use of shale oil products in military aviation and ship equipment; use of coal liquids in boilers; and testing of methanol and methanol-gasoline blends in auto engines and use of coal and shale-derived fuels in stationary diesel engines.

- Many synfuel developers appear to have in-house synfuel testing programs; the emphasis of these programs is primarily on synfuel characterization and not on end use testing. The data generated in these programs are generally considered company proprietary and are not published.

- Nearly all the refined shale oil products which have been used in combustion testing to date have been from the refining of the 100,000 barrels of Paraho shale oil at Sohio's Toledo (Ohio) refinery. Since this refining operation apparently did not involve the use of typical unit operations which would be employed in commercial refining of shale oil, the refined products from this operation are not considered to be representative of products from any future commercial refining of the shale oil.

- To date the synfuel testing effort has been severely curtailed by lack of adequate quantities of fuel for testing. Some of the planned testing programs will utilize shale oil products from the forthcoming refining of 50,000 barrels of shale oil by Union Oil for the Defense Fuel Supply Center.

- Synfuel products (especially the shale-derived materials) which will be marketed in the future will most likely be blends and not 100 percent pure products. The use of 100 percent pure products in the initial synfuel testing programs has been justified on grounds that it would simulate a possible "extreme/worst" case condition (at least from the standpoint of emissions and their environmental implications).

- Although the performance testing is continuing, the limited data which have been gathered to date indicate that the tested synfuels are generally comparable to petrofuels and do not present any unique problems from the standpoint of fuel handling and combustion characteristics. Potential problems with long-term fuel storage stability (observed with certain shale- and petroleum-derived middle distillates) and durability and material compatibility problems (e.g., possible increase in the engine wear with methanol use) are under investigation.

- The very limited data which have been collected on the emission of criteria pollutants (particulates, NO_x, SO_x, etc.) indicate that, except for a higher emission of NO_x with synfuels having a higher content of fuel-bound nitrogen, the emissions of such criteria pollutants are similar for both synfuel and their petrofuel counterparts. For most synfuels, however, no data have been collected on emissions of non-criteria pollutants such as polycyclic organic matter (POM's), primary aromatic amines, nitropyrenes and other organics. There is also very limited data on overall trace element composition of emissions.

ACKNOWLEDGMENTS

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The synfuel end use testing compendium is based on information and documents provided to the study by individuals/organizations engaged in synfuel characterization and end use testing; gratitude is expressed to the supporting individuals/organizations, particularly those in Table 1, to whom the project is deeply indebted.

EXAMPLE DATA SHEET NO. 1

COMBUSTION AND EMISSION CHARACTERISTICS OF COAL-DERIVED LIQUID

1. FUELS TESTED

Synfuels: SRC-II fuel (5 ratios of medium and heavy boiling range components); H-Coal (syncrude mode of operation, full-range distillate); EDS (full-range distillate).

Reference fuel: No. 6 and No. 2 petroleum-derived fuels.

2. TEST EQUIPMENT

An 80-HP firetube boiler system extensively modified to simulate a utility boiler including an indirectly fired air preheater, a scaled-down utility boiler burner, radiation shields to increase the thermal environment in the combustion chamber, and capabilities to implement staged combustion.

3. TEST SITE

KVB Combustion Research Laboratory, Tustin, California.

4. TEST OBJECTIVES

- Develop an understanding of the effect of compositional variations of a particular coal liquid and the resulting effects on the implementation of combustion modifications for pollutant emission reductions;
- Establish an understanding of the difference in the combustion and emission characteristics of coal liquids produced from various processes--specifically the SRC-II Process, the Exxon Donor Solvent Process, and the H-Coal Process;
- Establish a standard test method, using a small-scale facility, to predict the response to changes in operation of smoking tendency, CO, and NO_x. This will be used to differentiate various fuel properties and the performance of each fuel in a large variety of commercial boilers.

5. SPONSORING AGENCY

Electric Power Research Institute (EPRI)
Power Generation Program
Advanced Power Systems Division
Palo Alto, California

EPRI Project Manager: W.C. Rovesti
Telephone No: 415-855-2519

6. CONTRACTOR

KVB Inc.
Irvine, California

Principal investigators: L.J. Muzio, J.K. Arand
Telephone No. 714-641-6200

7. TEST CONDITIONS

A systematic set of experiments was conducted which investigated the following variables: excess air with single stage combustion, burner stoichiometry with two-staged combustion, firing rate, air preheat temperature, fuel temperature (viscosity), and atomizer (mechanical, steam).

8. ENVIRONMENTAL MONITORING

O_2, CO_2, CO, NO, SO_2, SO_3, unburned hydrocarbons, smoke number, particulate size distribution.

9. PROJECT STATUS

Completed.

10. RESULTS

Emissions from the various synfuels combustion tests in this program are summarized in Table A. A brief description of other emission test results are shown below.

SRC II

Particle size data indicate that SRC-II fuel blends produced finer-size-distribution particulate than No. 6 oil, the exception being SRC-II heavy distillate component under single-stage combustion. Measured SO_2 emissions were consistent with the fuel sulfur content, with nearly all fuel sulfur emitted as SO_2. An SO_3 concentration of 2 ppm for heavy distillate component was the only SRC-II test detecting this pollutant. Reference fuel No. 6 oil burn test also emitted 2 ppm SO_3. Unburned hydrocarbon concentrations measured for SRC-II combustion tests ranged from 1 to 14 ppm.

H-Coal

Average particle size of particulate matter proved to be less than 0.4 microns. Measured SO_2 emissions were consistent with fuel sulfur content in that the SO_2 emissions were the lowest of all synfuels tested. SO_3 was not detected. Unburned hydrocarbon emissions ranged from 1 to 4 ppm.

EDS

Two particle sizing tests showed the average particle size to be less than 0.4 microns. Measured SO_2 emissions were consistent with the fuel sulfur content. EDS flue gas samples showed no detectable levels of SO_3. Measured unburned hydrocarbon emissions were 1 and 2 ppm.

11. REFERENCE

Muzio, L.J. and J.K. Arand. Combustion and Emission Characteristics of Coal-Derived Liquid Fuels. EPRI AP-1878, Electric Power Research Institute, Palo Alto, Calif., 1981.

TABLE A. SUMMARY OF EMISSIONS

Fuel Type	Fuel Ash Content $lb/10^6$ Btu	Single-Stage			Two-Stage (Low O_2)			Two-Stage (High O_2)		
		O_2 %	Part. $lb/10^6$ Btu	NO ppm @ 3% O_2	O_2 %	Part. $lb/10^6$ Btu	NO ppm @ 3% O_2	O_2 %	Part. $lb/10^6$ Btu	NO ppm @ 3% O_2
No. 6 oil	0.0045	3.7	0.024	270	3.6	0.037	199	-	-	-
SRC-II 5.75/1	0.0017	3.8	0.014	400	3.2	0.022	303	4.9	0.020	382
SRC-II Medium Distillate	0.0012	4.0	0.011	476	3.1	0.017	307	4.2	0.012	342
SRC-II 2.9/1	0.0041	3.3	0.012	361	2.9	0.015	308	4.5	0.017	371
SRC-II 0.4/1	0.018	3.4	0.031	509	3.3	0.039	279	4.7	0.039	375
SRC-II Heavy Distillate	0.034	3.3 3.8	0.029 0.037	381 392	3.5	0.184	249	4.6	0.090	269
SRC-II Heavy Distillate (210°F Fuel Temperature)	0.034	-	-	-	3.2	0.065	339	-	-	-
H-Coal	0.0095	2.8	0.022	247	3.1	0.037	226	4.95	0.034	202
EDS fuel	0.0045	2.8	0.022	259	3.2	0.0184	270	5.15	0.0154	216

EXAMPLE DATA SHEET NO. 2

EFFECT OF FUEL BOUND NITROGEN ON OXIDES OF NITROGEN EMISSIONS FROM A GAS TURBINE ENGINE

1. FUELS TESTED

Synfuel: JP-5 type fuel derived from crude shale oil.

Reference fuel: JP-5 derived from petroleum.

2. TEST EQUIPMENT

Allison T63-A-5A turboshaft engine (free turbine type used in Army OH-58A and Navy TF-57A helicopters).

3. TEST SITE

Naval Air Propulsion Test Center
Trenton, New Jersey

4. TEST OBJECTIVES

- Confirm the presence of high levels of NO_x in engine exhaust;
- Obtain information on conversion efficiency of fuel bound nitrogen into NO_x;
- Assess the impacts of high nitrogen fuel on meeting pollution control regulations.

5. SPONSORING AGENCY

Deputy Chief of Naval Material (Development)
Department of the Navy
Washington, D.C. 20361

Project Officer: L. Maggitti
Telephone No: 202-545-6700

6. CONTRACTOR

Naval Air Propulsion Center
Fuels and Fluid Systems Division, PE71
Trenton, New Jersey 08628

Authors: A.F. Klarman, A.J. Rollo
Telephone No.: 609-896-5841

7. TEST CONDITIONS

The T63-A-5A engine was installed in a sea level test cell using a three-point mounting system. A flywheel and an Industrial Engineering Water Brake, Type 400, were connected to the engine gearbox assembly at the forward power output pad to absorb the engine power. The brake reaction was measured by a Baldwin load cell. All parameters to determine the engine starting and steady-state performance with the fuels were measured using standard test cell instrumentation. Engine performance data is contained in the reference report.

Fuels of varying nitrogen content were tested in a T63-A-5A engine to measure their effects on exhaust gas emissions. Five test fuels varying in fuel bound nitrogen content from 3 μg (nitrogen)/g (fuel) to 902 μg (nitrogen)/g (fuel) were evaluated. The nitrogen content in the fuel was adjusted by mixing a JP-5 type fuel derived from shale oil (902 μg (nitrogen)/g (fuel)) and regular petroleum JP-5 fuel (3 μg (nitrogen)/g (fuel)).

8. ENVIRONMENTAL MONITORING

Hydrocarbons, carbon dioxide, carbon monoxide, and nitrogen oxides.

9. PROJECT STATUS

Project report completed November 1977. This is part of an ongoing Naval program to evaluate fuel products derived from alternate sources.

10. RESULTS

Table B shows the results of the exhaust gas measurements performed during the test program. Additional results include the following:

- NO_x emissions for the same engine power rating increased with increasing fuel nitrogen content.
- The conversion efficiency of fuel bound nitrogen to NO and NO_x was approximately 45 percent for the test data in which the NO and NO_x values could be accurately measured.
- No significant effects were noted on engine performance or carbon monoxide (CO) and unburned hydrocarbons (HC) emissions due to the presence of high levels of fuel bound nitrogen.
- The use of shale derived JP-5 fuel with a high nitrogen content will make it more difficult to meet the EPA NO_x standards for aircraft gas turbine engines.

11. REFERENCE

Klarman, A.F. and A.J. Rollo. "Effect of Fuel Bound Nitrogen on Oxides of Nitrogen Emission From a Gas Turbine Engine", Naval Air Propulsion Center, Trenton, New Jersey, NAPC-PE-1, November 1977, 32 pp.

TABLE B. EMISSION DATA SUMMARY

Fuel Nitrogen μg/g fuel	Engine Power Rate	CO_2	CO			NO			NO_x (as NO_2)			HC			F/A
			ppm	g/s	g/kg fuel	ppm	g/s	g/kg fuel	ppm	g/s	g/kg fuel	ppm	g/s	g/kg fuel	(calculated)
3	IDLE	1.98	1035	0.714	99.2	6.7	0.00495	0.688	6.7	0.00690	1.06	157	0.0503	6.99	0.00979
	60% NR	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	MIL	3.03	140	0.227	9.25	23.9	0.0416	1.69	23.9	0.0637	2.59	5.6	0.00422	0.172	0.0146
47	IDLE	2.08	985	0.692	90.5	7.7	0.00579	0.758	7.3	0.00887	1.16	131	0.0427	5.59	0.0105
	60% NR	2.43	430	0.482	35.0	12.7	0.0152	1.11	13.1	0.0241	1.75	18.3	0.00952	0.692	0.0119
	MIL	3.03	130	0.207	8.60	24.3	0.0415	1.72	24.3	0.0635	2.64	8.4	0.00621	0.258	0.0146
267	IDLE	2.08	1005	0.698	92.3	9.1	0.00677	0.895	9.4	0.0108	1.42	134	0.0432	5.71	0.0105
	60% NR	2.43	380	0.438	31.0	16.5	0.0204	1.44	16.7	0.0315	2.24	14.5	0.00775	0.549	0.0119
	MIL	3.03	140	0.224	9.26	27.6	0.0473	1.96	27.6	0.0726	3.00	11.1	0.00825	0.341	0.0146
515	IDLE	2.10	950	0.688	86.7	11.6	0.00900	1.13	12.3	0.0146	1.85	109.6	0.0368	4.65	0.0106
	60% NR	2.43	445	0.482	36.2	17.8	0.0206	1.55	18.4	0.0327	2.47	18.6	0.00935	0.702	0.0119
	MIL	3.03	130	0.210	8.60	31.6	0.0547	2.24	31.6	0.0838	3.44	8.7	0.00652	0.267	0.0146
902	IDLE	2.10	992	0.710	90.4	14.9	0.0114	1.45	16.0	0.0188	2.39	116	0.0385	4.91	0.0106
	60% NR	2.43	460	0.500	37.4	22.1	0.0257	1.92	22.5	0.0401	3.01	18.2	0.00918	0.687	0.0119
	MIL	3.03	135	0.218	8.93	35.9	0.0621	2.55	36.3	0.0962	3.95	8.4	0.00629	0.258	0.0146

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COMPARATIVE TESTING OF EMISSIONS FROM COMBUSTION[†] OF SYNTHETIC AND PETROLEUM FUELS

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EMISSIONS FROM COMBUSTION OF SYNTHETIC FUELS

There are two basic reasons to investigate the emissions from the combustion of coal- and shale-derived synthetic fuels:

- The physical and chemical characteristics of these synfuels will probably be different from the petroleum-based analogs that they will replace or supplement (e.g., by blending); therefore, the emissions from their burning are likely to be different.
- The types and numbers of combustors in which synfuels might be used are very large; therefore, the potential for exposure to their emissions is very great.

These two reasons argue for research and development now, before extensive commercialization of synfuels, on procedures that can be used to test emissions from representative combustors burning prototype synfuels, and petrofuels that they may replace. Once developed, such procedures can be used to determine which synfuel/combustor combinations should be avoided, and which combinations will result in "clean" emissions (perhaps cleaner than from present combustion of petroleum-based fuels, or from future combustion of lower-grade petrofuels).

CHARACTERISTICS OF SYNTHETIC FUELS

Both physical and chemical characteristics of fuels can affect combustion emissions. Physical properties of solid and liquid fuels such as particle size, density, viscosity, and surface tension affect the rate at which the fuel volatizes to a combustible (gaseous) state. Many of the solid and liquid products available to date from U.S. synfuel pilot plants have physical properties that tend to make them volatize less easily than the coal and petroleum-based fuels they may replace.

Generally, the chemical properties of pilot-scale synfuels produced to date have also been of concern relative to petroleum analogs, mainly because of their greater concentration of high-molecular-weight organics. A considerable and growing literature exists on the content of aromatic and substituted aromatic components of coal- and shale-based synthetics (e.g., reference 1). There are, however, many process options for producing clean synfuels such as methanol, or refining crude products to specifications meeting or exceeding those for current petroleum fuels.

There is, therefore, a trade off between cleaning the synthetic product before combustion and burning the fuel cleanly. Aside from consideration of fuel handling and distribution concerns, the degree of need for a clean fuel will depend on the combustion application.

THE POTENTIAL POPULATION OF SYNFUELED COMBUSTORS

Emissions are greatly affected by type of combustor and how well it is being operated. Light oil, wood, and even methane can lead to undesirable emissions if they are burned improperly. Aside from the tens of millions of mobile internal-combustion engines that are candidates for synthetic fuels (or blends with petrofuels), many stationary units in this country are presently fired with oil:

- Thousands of large utility boilers.
- Hundreds of thousands of industrial and commercial boilers.
- Hundreds of thousands of stationary diesel engines.
- Millions of commercial and residential furnaces.

There are certainly examples of both "clean" and "dirty" burning units in each of the above categories. Generally speaking, however, the amount of attention given to the operation of the units decreases from top to bottom of the list. Typical combustion efficiency of units in each of the four categories probably follows the same order.

On the other hand, fuels burned in residential and commercial furnaces are generally lighter and cleaner than those in diesels, which in turn are lighter and cleaner than those burned in industrial boilers. Overall, large utility boilers most frequently burn the heaviest fuels of all.

This apparent inverse relationship between attention to operation and cleanliness of fuel leads us to suspect that the primary categories of concern among stationary sources might be the middle two -- industrial/commercial boilers and stationary diesels. Also, a recently completed study on synfuels uses (reference 2) tends to indicate that these two categories are likely to be among the first stationary sources to use synfuels in commercial quantities.

EPA therefore initiated a research and development program early this year to develop a set of engineering procedures for comparative testing of emissions from combustion of coal- and shale-based liquid synthetics and petroleum-based analogs. It is designed to be a multi-phased program with several iterations of procedure development, followed by combustion tests to hone the procedures. The following sections of this paper describe the current status of the initial work (Phase I) of this program.

EXISTING EMISSIONS DATA

Data on emissions from combustion of synfuels are very limited. Data on combustion products from oil burning, especially organics, are also limited. Whereas emissions of inorganics are fairly predictable as oxidation products of fuel constituents, organic products of incomplete combustion are a different story. The possibilities are virtually limitless and much more difficult to predict; carefully collected empirical data are needed.

Because changes in emissions are of greater concern than absolute emission rates when switching to synthetics, data of greatest value will be comparative data on emissions from a synfuel and its petroleum analog(s), burned in an appropriate combustor at representative operating conditions. One reason is the oft-stated observation that emissions from combustion of currently burned petroleum fuels constitute an accepted baseline. Another reason is that physical, biological, and chemical characteristics of synthetic fuels (and their emissions) will be evolving as the synfuel industry evolves. It will therefore be important to continually combustion-test emerging synthetic fuels to understand the best environmental and economic balance between cleaning these fuels and burning them cleanly.

PROCEDURES FOR COMPARATIVE TESTING OF EMISSIONS

After several months of Phase I of the EPA program, a very preliminary set of procedures has been developed that addresses personnel safety, combustor operation, emissions sampling, and sample analysis. An overview of current thoughts on each of these aspects follows.

PERSONNEL SAFETY

Because of the hazardous nature of some of the fuels, samples, and residues being handled, precautions are being taken to protect technicians, supervisory personnel, and observers. The materials requiring greatest attention are spills of synthetic and heavy petroleum fuels, residues from cleaning the combustor, and the collected samples of combustion products. During combustion runs and combustor cleaning operations, specified disposable protective clothing and cartridge respirators must be used. Personnel involved in sample handling, preparation, and analysis are required to follow standard precautionary laboratory procedures.

COMBUSTOR OPERATION

The following considerations are especially important for development of procedures for comparative testing of synfuel combustion emissions:

- A combustor that is representative of intended uses must be used. This will generally preclude use of laboratory-scale burners, and will often require combustors with substantial fuel feed rates.

- Large quantities of the synfuels to be tested will often not be available. This will dictate relatively short combustion runs.

- Run-to-run cross-contamination of internal combustor surfaces is a potential problem that may confuse emission measurement results. Some method of equipment cleaning between runs needs to be developed.

With these three factors, plus other considerations derived from a knowledge of how combustors and their operation affect emissions, a preliminary set of procedures, summarized below, has been established:

1. Clean combustor surfaces. This step will consist of brushing and vacuuming accessible internal surfaces to remove loose deposits from the previous run. This step also applies to the dilution tunnel discussed later.

2. Burn No. 2 oil. A typical No. 2 fuel oil, available in sufficient quantity to be used as a reference fuel for all runs, will be used for approximately 1 hour to bring the combustor to steady operation and "recondition" the internal surfaces.

3. Burn test fuel. The fuel supply will be switched to the synthetic or petroleum fuel to be tested. Each test burn is expected to last 2 to 6 hours.

4. Shut down the combustor, and repeat cycle. Eventually, it is hoped to be able to complete one run (steps 1-3) per day or four runs per week. It remains to be seen, of course, whether stable operation and repeatable results can be obtained in sizable combustors with such short turnaround time.

The test fuel firing rate will be set at 80% load and the excess air adjusted to achieve 10% opacity or less in the stack gas from the boiler (excess air will generally be in the range 5%-10%). This opacity setting represents energy-efficient operation for oil-fired boilers. It also represents marginal performance from a particle emissions standpoint. Differences between fuels in emissions potential will therefore tend to be accentuated at this setting, which should expedite screening for potential problems.

With some of the cleaner fuels, an opacity as high as 10% may not be attainable. In such situations, an excess air setting of about 5% is planned. If, for some of the heavier fuels, an opacity as low as 10% cannot be maintained at a reasonable excess air setting, control at about 35% excess air is planned.

The diesel engine will be operated at its continuous load setting of 165 kW (80% load). It will be operated at approximately 85% excess air, which is typical for such combustors, and the opacity measured but left to vary from fuel to fuel.

FUEL AND EMISSIONS SAMPLING

As shown on Figure 1, five types of samples are being taken during Phase I of the program. They are, briefly:

1. Fuel samples. Grab samples are taken from fuel storage (most of the fuels for Phase I of the program are stored in drums).

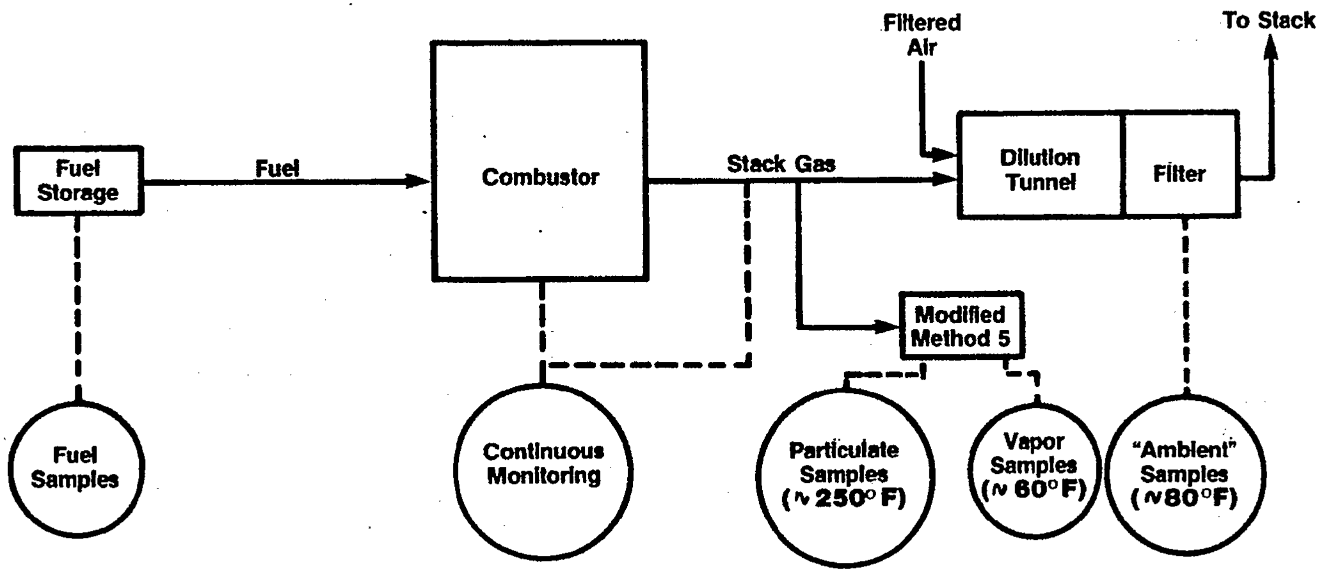


Figure 1. Sampling - Comparative Emissions Test Procedure (Phase I)

2. Continuous monitoring. Stack gas measurements of O_2, CO, CO_2, NO, NO_2, SO_2, total hydrocarbons, and opacity are made continuously while the conditioning No. 2 fuel and the test fuels are being burned.

3. Particulate samples. Particles in the stack gas will be sampled by a modified Method 5 train (Figure 2 and Reference 3). Particles will be collected in a fiberglass filter at approximately 125°-150°C (250°-300°F) over a 2- to 3-hour period during each run of a test fuel.

4. Vapor samples. Stack gas vapors that pass through the filter of the modified Method 5 train will be cooled to approximately 15°C (60°F) and collected on XAD-2 sorbent material. Vapor samples will be collected over the same periods as the particulate samples.

5. "Ambient" samples. A portion of the stack gas from the combustor will be mixed with filtered air in a dilution tunnel (air-to-stack gas ratio of approximately 10:1). A large (50-cm square) Teflon-coated fiberglass filter at the end of the dilution tunnel will collect particles during the full length of each run of a test fuel.

The dilution tunnel is included in the preliminary procedures for two reasons: (a) by simulating atmospheric dilution/cooling conditions near the exit of the stack, it provides a sample more representative of ambient particles than the ones collected in the stack, and (b) it is an inexpensive way to collect relatively large samples for both chemical and biological testing.

FUEL AND EMISSIONS ANALYSES

Figure 3 summarizes the physical, chemical, and biological analyses being done on the samples of fuels, stack gas particles, stack gas vapors, and simulated "ambient" particles from the dilution tunnel. The primary details of the preliminary analytical procedures follow.

1. Fuel specifications. Standard ASTM procedures are being used to measure the fuel parameters of most common interest to people who purchase or burn fuels. The following measurements are also made for each fuel: inorganic screening by spark source mass spectrometry (SSMS), gas chromatography-mass spectrometry (GC-MS)for qualitative organic screening, spot test for polycyclic aromatic hydrocarbons (PAHs), and boiling point analyses for organics between 100°-300°C and >300°C.

2. Inorganics. Elemental constituents in the fuels will be semi-quantitatively screened by SSMS. Elements selected from the fuel screening will be analyzed in the stack gas and "ambient" particles by atomic absorption (AA).

3. Organics. The objective for analysis of organics, as for inorganics, is to screen for major compositional differences between samples from synthetic fuels and from their petroleum analogs. The battery

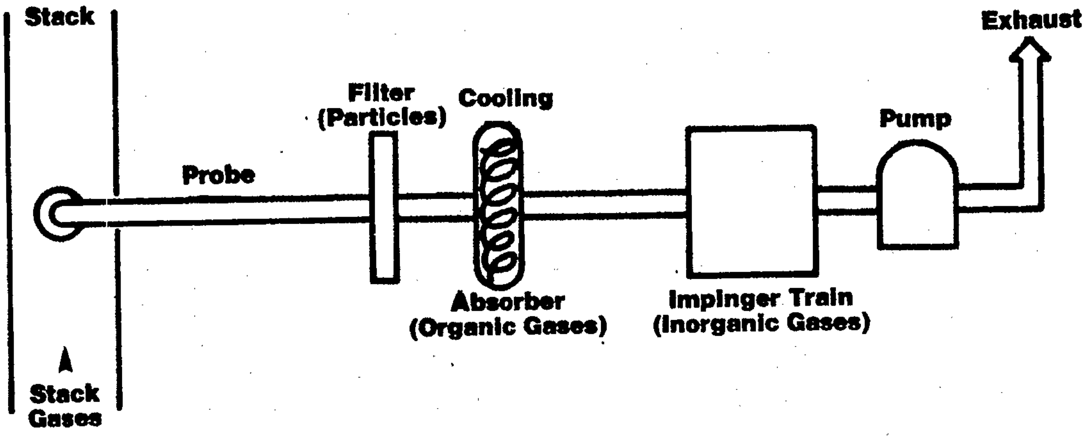
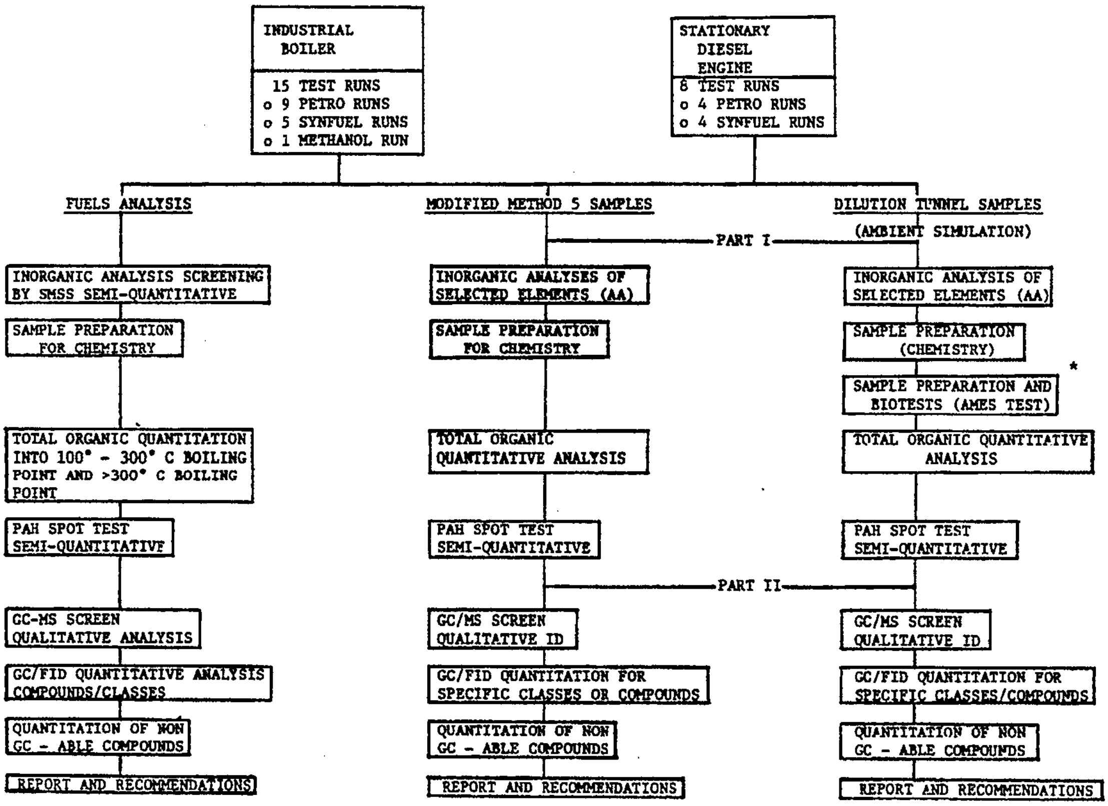


Figure 2. Modified EPA Method 5 Train



*Bioassay Screening - Based on 200 mg particulate sample (20 mg organic extractables).

Figure 3. Analyses - Comparative Emissions Test Procedure (Phase I)

of techniques includes (a) quantitation of total organics; (b) the "spot" test (reference 4) for PAHs; (c) a qualitative screening by GC-MS, to obtain a very rough "fingerprint" of the organic emissions; and (d) quantitation of the non-gas-chromatographable portion. Samples that are compositionally distinctive, based on the above tests, will be further analyzed by gas chromatography-flame ionization detection (GC-FID) to obtain semi-quantitative information on major classes or compounds present.

All three emissions samples -- stack gas particles, stack gas vapors, and "ambient" particles -- will undergo this battery of tests. The fuels will be analyzed similarly.

4. Bioassays. Comparative biological screening of emission samples in Phase I of the program will be limited to short-term bacterial mutagenicity tests of the type originally developed by Ames. The minimum desirable sample quantity for these tests is 20 mg of organic extractables. If the extractables constitute 10% of the total weight of particles collected, a minimum of 200 mg of particulate catch will be required for the bioassays alone. This amount of sample can only be obtained on the filter at the end of the dilution tunnel, with current procedures. In fact, several of the planned runs with relatively clean fuels are not expected to produce sufficient sample for biological screening. Runs with sufficient sample will be tested using the *Salmonella typhimurium* strain TA98, reverse mutation assay. Each test will be run at 5 to 7 dose levels, both with and without metabolic activation. Any testing beyond this simple assay, such as assays on fractions of samples, will be done only as screening indicates a need and as sample material allows. The need for more extensive biological testing (e.g., additional mutagenesis assays or carcinogenesis assays) in future phases of the program will be determined largely from the results of Phase I.

COMBUSTION EMISSIONS TESTING

A series of comparative combustion emissions tests has been planned as part of Phase I of the program, to evaluate the soundness and practicality of the preliminary testing procedures. The following sections describe the combustors to be used, the fuels to be burned, and the schedule for the remainder of Phase I.

COMBUSTORS

Table 1 lists the characteristics of the two combustors being used at EPA's combustion research facility at the Research Triangle Park, NC. The package boiler (so-called because units of this size can be shop-fabricated and delivered to the site as a "package," rather than being erected at the site) represents small-to-medium-sized fire-tube boilers used in industry and commercial establishments. In addition to its normal dual-fuel burner, it can be (and has been, in past experiments) equipped with a "low-NO_x" burner which promotes staged combustion and lower emissions of NO_x. In Phase I, the conventional burner will be used; in subsequent phases, the effectiveness of the

Table 1. Combustors Being Used in Comparative Emissions Tests (Phase I)

PACKAGE BOILER

- North American scotch marine boiler
- Typical of a broad range of small-to-medium industrial and commercial boilers
- Capacity: 2.5×10^9 kJ/hr fuel rate (2.5×10^6 Btu/hr fuel rate; 2,000 lb/hr steam)
- Operating rate: 80% of capacity; approximately 50 liters per hour (13 gal./hr) of fuel
- Dual-fuel burner (heavy oil and gas)
- Outside dimensions: 1.4 meters (4-1/2 ft) diameter, 3 meters (10 ft) long

STATIONARY DIESEL

- Caterpillar Model D334
- Typical of medium-sized industrial stationary engines
- Capacity: 205 kW (generator output)
- Operating rate: 80% of capacity; approximately 53 liters per hour (14 gal./hr) of fuel

new low-NO_x burner design may be tested on synfuels.

The stationary diesel represents medium-sized industrial and commercial engines used for backup power generation, pumping applications, and powering various other mechanical equipment. Both combustors will be operated as described in the previous section on "Combustor Operation."

Future phases of the program are expected to repeat tests with these combustors for various load and operating settings. In addition, tests may be run with the low-NO_x burner to determine its effect on synfuel combustion emissions. Another possibility is a series of tests on residential furnaces.

FUELS

The fuels used in Phase I testing were chosen to cover a broad range of petroleum and synthetic products. This is mainly to check the applicability of the test procedures. A secondary purpose is to obtain information on major differences in emissions among fuels. It is important to understand that, whereas the coal- and shale-based synthetics being used are typical of those currently available in the U.S. in barrel quantities, they may not be at all typical of synthetics that are eventually marketed for use in industrial boilers and stationary diesels. Therefore, whereas the results from Phase I will be useful in refining the test procedures and planning for Phase II testing, they are not intended for use in environmental assessment of synfuel combustion.

Table 2 lists the fuels being combusted. Additional descriptions follow.

1. Petroleum fuels. Seven petroleum fuels will be tested -- six in the package boiler, and three in the diesel, with two of the seven burned in both units. Four of the fuels will be heavy (No. 6 grade), with sulfur contents ranging from 1 to 3%, nitrogen 0.04 to 0.7%, and ash 0.05 to 0.3%. The other three fuels are lighter (No. 2 grade) with sulfur contents of 0.02 to 0.5%, nitrogen 0.04 to 0.1%, and <0.1% ash. All seven fuels were obtained from east coast distributors.

2. Coal-derived distillates. Three different coal-derived synthetics will be tested. An SRC-II heavy distillate from the Ft. Lewis Solvent Refined Coal pilot plant and an EDS middle distillate from the Exxon Donor Solvent pilot plant in Baytown, Texas, will be burned in the package boiler. The EDS middle distillate and an SRC-II middle distillate will be burned in the stationary diesel.

3. Shale-derived fuel. Refined product (light No. 2) from the Sohio refinery run of Paraho shale oil will be burned in both the package boiler and diesel. This oil has been heavily hydrotreated, and appears to be one of the cleanest fuels to be burned in Phase I.

Future phases of the program are planned to repeat burns with these fuels, other petroleum fuels, other synthetic fuels as they become available, and blends of synthetics and petrofuels.

Table 2. Fuels Being Used in Comparative Emissions Tests (Phase I)

PACKAGE BOILER	RUNS
o 4 Heavy Petroleum Fuels	6
o 2 Light Petroleum Fuels	3
o 1 Coal-Derived Middle Distillate	2
o 1 Coal-Derived Heavy Distillate	2
o 1 Shale-Derived No. 2 Fuel	1
o 1 Methanol	1
	15
STATIONARY DIESEL	
o 3 Light Petroleum Fuels	4
o 2 Coal-Derived Middle Distillates	3
o 1 Shale-Derived No. 2 Fuel	1
	8

Two of the light (No. 2) petroleum fuels, one of the coal-derived middle distillates, and the shale-derived No. 2 fuel are identical for both combustors.

SCHEDULE

The series of combustion emission tests just described will be conducted during November and December of this year. The bulk of the samples will be analyzed from January through March 1982. Data will be compiled and distributed to program participants and fuel suppliers during early spring. A workshop for discussion of data interpretations, test procedure revisions, and plans for Phase II of the program is planned for June 1982. The workshop will bring together EPA and DOE participants, fuel suppliers, and selected additional experts in combustion, analytical chemistry, and data analysis.

SUMMARY

As coal- and shale-derived synthetic fuels begin to enter the market in the 1980s, questions will arise regarding the nature of the emissions from their combustion. A program was recently initiated by EPA to develop engineering procedures for measuring emissions so that concerned parties (EPA, synfuel developers, synfuel users, and others) can address such questions.

The basic approach that has been taken is to compare emissions from synfuels burning to emissions from the burning of petroleum-derived fuels that will be displaced, in combustors that are representative of expected synfuel applications. An important objective of the program is to devise testing procedures that are as simple and inexpensive as possible, but that highlight important differences in emissions from synfuels and petrofuels, where they exist.

The program for development of procedures for making such tests will be multiphased, over a several-year period. Preliminary procedures have been developed for liquid-fueled industrial boilers and stationary diesels. Combustion testing is now underway to check the feasibility and practicality of the procedures. The procedures and data from the first-phase results will be reviewed at a workshop by program participants and additional experts. Subsequent phases of the program will focus on refinement of the procedures and expansion of their applicability to other fuel/combustor combinations.

* * *

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Many people in the Environmental Protection Agency have been involved in the planning of this program, and many more are expected to contribute as the program matures. The authors especially appreciate the contributions to date of: Michael C. Osborne and Jack H. Wasser of the Combustion Research Branch, Raymond G. Merrill of the Technical Support Staff, and Robert P. Hangebrauck of the Energy Assessment and Control Division, all of the Industrial Environmental Research Laboratory, RTP; Joellen Lewtas of the Health Effects Research Laboratory, RTP; and Donald Barnes and Carl Mazza of the Office of Toxic Substances.

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