Distribution Category:
Coal Conversion and Utilization--
Liquefaction (UC-90d)

ANL-79-77

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REVIEW AND ANALYSIS OF SPRAY COMBUSTION AS
RELATED TO ALTERNATIVE FUELS

by

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Performed under DOE Intra-agency Agreement
DE-A122-79PC 20074 for
Pittsburgh Energy Technology Center

September 1979

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ABSTRACT

A review was conducted during the period of mid-June to mid-August 1979, of the literature on spray combustion. Particular attention has been paid to theoretical and experimental work on droplet and spray combustion applicable to the use of alternate fuels, mainly liquid fuels derived from coal and shale. The Argonne National Laboratory technical information center and computerized information-retrieval systems have been extensively used in this effort. Sixty-two sponsored research programs have been identified as pertinent to the problems of spray combustion. Conversations were had with twenty-one nationally recognized authorities in the field of spray combustion to assist in evaluating the literature and research needs for alternate fuel utilization. Recent reports of alternate liquid fuel spray-combustion demonstration tests have been reviewed and discussed. Problem areas associated with the combustion of alternate liquid fuels have been identified.

I. SUMMARY

A review was conducted during the period of mid-June to mid-August 1979, of the literature on spray combustion, with particular emphasis on theoretical and experimental work on droplet and spray combustion relevant to the use of alternate fuels* (mainly liquid fuels derived from coal and shale).

Principal differences between coal-derived liquid fuel and petroleum have been identified. Coal liquids have a lower hydrogen-to-carbon ratio, higher aromatic compound content, greater tendency to form soot, and burn with a more luminous flame. Coal liquids pose potential carcinogenic hazards in handling the fuel and from soot resulting from their combustion. Coal liquids are less stable than petroleum, contain considerably more organic nitrogen, produce more NO_x when burned, and contain less sulfur. They also contain a broader range of volatiles, and spray droplets of coal liquids undergo swelling, disruptive boiling, microexplosions, liquid-phase pyrolysis, and have greater radiative effects.

Although demonstration tests have shown that coal liquids can be burned in various combustors, such as gas turbines, diesel engines, utility boilers, and residential furnaces, these tests have identified problems that

*The terms alternate fuel, alternative fuel, and synfuel are used in current literature and in this report synonymously.

may be encountered in combusting these fuels. Major problems identified are plugging and fouling of fuel nozzles, increased NO_x emissions, hot corrosion of turbine blades, cooling-hole plugging, irregular burning, higher combustor-wall temperatures, greater soot formation, and variability between coal-liquid samples.

A literature survey has shown that, although considerable progress has been made in understanding the spray-combustion processes of "normal" petroleum liquids, considerable research work is needed in the area of spray combustion of alternate fuels. Furthermore, the literature indicates that spray combustion of fuels similar to coal liquids is considerably more complex than spray combustion of "normal" petroleum stocks, and that a major research effort is required in anticipation of significant substitution of coal liquids for imported petroleum fuels in the United States.

The literature review and communications with over 20 nationally recognized researchers in spray combustion have identified problem areas and technological needs associated with the utilization of alternate liquid fuels to supplement domestic petroleum supplies. Briefly, the identified needs are:

1. Development of both a technological data base and design simulation models for suppliers of industrial combustion equipment.
2. Development of integrated programs within which experimental studies can be made in environments that are controlled and yet are representative of those encountered in current and future combustors.
3. Continuous development and application of theoretical models of both the global and detailed type.
4. Exploitation of stirred-reactor technology for the characterization of the behavior of recirculation zones with intense backmixing.
5. Quantitative understanding of primary atomization and secondary shattering of droplets in turbulent flow.
6. Chemical kinetic studies of the pyrolysis and oxidation of aromatics, particularly aromatics containing nitrogen.
7. Investigation of turbulent flames in configurations that allow a systematic progression in complexity, starting with premixed and/or prevaporized systems and proceeding to flames with direct liquid injection.
8. Studies of the collective intercoupling of droplets turbulent flow and chemical kinetics.
9. Specific research in the areas of formation and emission of soot, NO_x , and polycyclic organic matter.

10. Studies of the effects of fuel additives and emulsions on ignition and combustion characteristics, and the formation of pollutants.
11. Studies of the corrosion and erosion effects on combustors of alternative fuel spray combustion.
12. Development of improved instrumentation diagnostics, with emphasis on steady-state temperature measurements in a real system with laser diagnostics.

II. OBJECTIVES

The objectives of this report on droplet and spray combustion relevant to the combustion of synfuel* liquids are:

1. To evaluate the relevance of past published work on droplet and spray combustion to the combustion of synfuel liquids (shale oil and coal-derived liquids), and heavy petroleum and residual oils.[†]
2. To identify information gaps and propose theoretical and experimental work needed for practical combustion of synfuel liquids.

III. INTRODUCTION

Over a century ago, it was discovered that the atomization of fuel oils provided a convenient means of obtaining self-sustaining flames. Considerable practical technology evolved early in this century concerning spray combustion of fuel oils in domestic and industrial furnaces. However, little understanding of the process was acquired. With the advent of aircraft gas turbines and liquid-fueled rockets, the emphasis changed and extensive research programs were devoted to the combustion of the lighter fuels, such as aviation gasolines and kerosenes. Consequently, one-dimensional models of spray-combustion chambers have developed to the point where they can be used for the design of steadily operating, large, multi-injector liquid rocket engines.¹ However, design and construction of boilers, kilns, and furnaces have not had the advantage of extensive research programs and have traditionally proceeded in an empirical fashion, and designs of new systems are simply variations of older models. This approach does not provide optimum design and can cause expensive and time-consuming delays in bringing new systems on line.

Recent escalation of this nation's dependence on imported oils has led to the promulgation of the Presidential Import Reduction Program (July 16, 1979), which proposed reduction of oil imports by six million barrels a day by 1990, with another reduction of 4.5 million barrels a day by year 2000. The

*Footnote, p. 1.

[†]Heavy petroleum and residual oils are considered within the scope of work for the alternate fuels combustion program.

program also plans to direct development of production facilities for 2.5 million barrels a day of oil substitutes by 1990. Furthermore, the program would require utilities to cut current oil consumption by 50% leading to a reduction in the use of petroleum stocks by 750,000 barrels a day.

Coal, our nation's most abundant fuel source, appears to be an alternative fuel to supplement domestic petroleum production and, in part, meet the goals of the Presidential Import Reduction Program. Coal can be burned as a solid or, after conversion, as either a liquid or gas. Coal gasification provides the most desirable fuel form; it is low in pollutant emissions, is easy to handle, and has good combustion characteristics. Unfortunately, coal gasification is relatively expensive. Although coal can be burned directly, it may not be economically feasible to provide the needed coal storage and handling facilities, environmental-control devices, and/or combustor modifications. Coal liquefaction provides a fuel that is easy to handle and one in which the potentially adverse characteristics are reduced.

In making liquid fuels from coal, it has been necessary to increase the hydrogen-to-carbon ratio of the fuel. Of the many different hydrogenation processes for coal liquefaction that have been evaluated, three processes have demonstrated potential as utility and commercial fuel sources. These are: SRC-II (solvent refined coal), H-Coal (Hydrocarbon Research, Inc.), and EDS (Exxon donor solvent). SRC-II is the most advanced in terms of physical scale--a DOE pilot plant at Tacoma, Washington is the pilot plant for coal liquefaction and produces 75 barrels of coal liquids per day. The H-Coal and EDS pilot plants should be in operation within two years.

During the 1980s, heavy petroleum oils, residual oils, and, to a limited extent, coal liquids are expected to be used in utility boilers and industrial boilers and furnaces where conversion to direct coal combustion is not practical. It is conceivable that by commercialization of one or more of the advanced liquefaction processes, such as SRC-II, H-Coal, and EDS, production of 450,000 barrels a day by 1990 and 900,000 barrels a day by 1995 is possible.

Our energy rich society has developed combustion technology that has not been overly concerned with fuel conservation in the past and certainly has not devoted much effort on synfuel liquid utilization. To utilize synfuel liquids in the most efficient and practical manner, a coordinated and integrated research and development program is needed in the area of synfuel liquid combustion technology.

IV. SYNFUEL LIQUID CHARACTERISTICS

The Electric Power Research Institute (EPRI) provided the following summary of some of the problems associated with the use of synfuel liquids:²

"If there is one generic problem common to SRC-II, H-Coal, and EDS, it is the lack of thorough, uniform, and authoritative data on the handling, storage, and (especially) combustion characteristics of coal liquid beneath steam boilers or in gas turbine combustors. Coal is a widely variable feedstock, depending on its geographic source, and a thoroughly representative range of types has not yet

been put through all the coal liquefaction processes. The spectrum of fuel samples is, therefore, limited. Some combustion tests have been made at laboratory scale, but much field testing will be needed to ensure that oil-fuel turbines and boilers can use the coal-derived distillates and heavier fuel grades with only modest equipment changes--or, better yet, none at all."*

The characteristics of coal and shale liquids could cause problems associated with combustors in gas turbines. Synfuel liquids are high in organically bound nitrogen, which, for the most part, is converted in the combustion process to oxides of nitrogen (NO_x). Synfuel liquids contain trace-metal contaminants that can lead to hot corrosion in turbine hot sections.³ Other problems associated with synfuel are its tendency to form soot owing to its high carbon-to-hydrogen ratio and aromaticity, its formation of a more luminous flame when burned, its potential health hazard due to the presence of polycyclic aromatic compounds, and its less stable storage characteristics. Furthermore, its multicomponent state, with widely differing volatilities and states of mixedness, presents problems to the combustor designer because of liquid droplet swelling, disruptive boiling, microexplosions, liquid-phase pyrolysis, and liquid radiation-absorption effects.

Table 1 presents a comparative example of fuel properties of synfuel liquids and middle and heavy distillates of petroleum fuel oils.

V. SYNFUEL LIQUID COMBUSTION DEMONSTRATIONS

Demonstration ignition and combustion tests have been conducted in recent years as samples of synfuel liquids have become available. These tests have ranged from single drop experiments by Jordan *et al.*⁵ to the burning of 4500 barrels of synfuel liquid in an existing utility boiler by Piper *et al.*⁶ Other tests have been conducted by Haebig and Davis⁷ in a residential boiler, and by Muzio and Arand⁴ in an 80-hp boiler. Quinlan and Siegmund³ report combustion tests of EDS in a 50-hp Cleaver-Brooks fire tube boiler. Clark *et al.*¹ and Cabal *et al.*⁸ have investigated the special problems of burning synfuel liquids in stationary gas turbines. Longwell⁹ has made an analysis of combustion problems that may be encountered in the utilization of synfuel liquids in transportation engines.

Some example comments by these investigators are:

1. Jordan *et al.*⁵ note that "the behavior of these coal extracts cannot be satisfactorily characterized by any 'oil based' constant" due to irregular burning and excessive swelling of synfuel droplets. "Special problems may, therefore, be encountered when burning the highly aromatic products of solvent extraction/hydrogenation of coal, particularly the heavier fractions and high boiling point SRC." Jordan goes on to note "that water emulsification could offer a practical solution" to smoke and particulate emission from large-scale oil-fired systems.

*The authors and some of the people consulted believe efficient and environmentally acceptable combustion of coal liquids will require appreciable change in combustion equipment.

Table 1. Typical Fuel Characteristics⁴

	Western Kentucky Coal	SRC-II	#6 Oil	#2 Oil
C, wt %	72.2	86.6	86.61	86.82
H, wt %	5.0	8.38	12.25	12.69
N, wt %	1.4	1.12	0.24	0.024
S, wt %	3.6	0.26	0.28	0.11
Ash, wt %	10.5	0.008	0.016	0.003
O ₂ , wt % (by difference)	7.3	3.63	0.6	0.35
Gross Heat of Combustion, Btu/lb	13,150	17,040	19,150	19,190
API Gravity	-	8.3	2.3	32.3
Viscosity, SSU @ 140 F (60°C)	-	35.6	324 (100 F) (38°C)	34

2. Piper et al.⁶ who investigated the combustion demonstration of SRC-II fuel oil in a tangentially fired boiler reported the following:

- "No major operational problems were encountered due to the combustion of SRC-II fuel oil. Visual inspections performed by Consolidated Edison indicated no evidence of deleterious effects on the pump used to feed SRC II-fuel oil to the test boiler.
- "Boiler thermal efficiency levels with SRC-II fuel oil were comparable to those obtained with No. 6 fuel oil.
- "The combustion of SRC-II fuel oil resulted in nitrogen oxide emission levels approximately 70% greater than those for No. 6 fuel oil under all test conditions. Higher NO_x emissions were anticipated for the SRC-II fuel oil due to its higher nitrogen content.
- "Nitrogen oxide reductions achievable through combustion modifications were on the order of 35% for both SRC-II and No. 6 fuel oils.

- "Particulate mass emissions were lower for the SRC-II fuel oil than for No. 6 fuel oil. The characteristics of the particulates were sufficiently different to suggest different formation mechanisms.
- "Total hydrocarbon emissions were less than 3 ppm under all operating conditions with both fuels.
- "The total polycyclic organic matter (POM) emissions for both fuels were low; less than 6×10^{-6} lb/10⁶ Btu. Although the emission levels with the SRC-II fuel were nominally higher than those exhibited by the No. 6 fuel oil, the measurement uncertainties are such that no significant trend can be assigned at this time. However, results of another study would indicate the POM emission levels measured on these liquid fuels are substantially below those measured on direct coal fired boilers."

3. Haebig and Davis⁷ note that while synfuel liquids produce negligible amounts of sulfur oxides, CO, and hydrocarbons, the emissions of NO_x were problematic. They suggest that removal of nitrogen from coal liquids by upgrading would solve this problem and that minimum processing requirements need to be ascertained.

4. Muzio and Arand,⁴ in reporting results of combusting synfuel liquids in an 80-hp boiler, make the following specific conclusions.

- "The combustion performance of the solvent refined coal oil is equivalent to that of typical utility type fuel oils. It is volatile (similar to #2 oil) and does not require preheating to achieve acceptable viscosity for pumping and atomization.
- "Potential problems with furnace slagging and metal wastage occasionally encountered with coal combustion should be negligible with SRC because of its low sulfur and ash contents.
- "Nitric oxide emissions could be maintained at about 0.4 lb/10⁶ Btu for the SRC utilizing combustion conditions typical of many large utility boilers. This was accomplished with two-stage combustion and 3% excess oxygen in the flue gas. At these conditions, low stack gas concentrations of carbon monoxide and particulates were maintained.
- "Nitric oxide emissions could be reduced below 0.3 lb/10⁶ Btu for SRC by blending SRC with other petroleum-based fuel oils having much lower fuel nitrogen and then firing with two stage combustion, or using a fuel additive

containing manganese and then firing with two stage combustion.*

- "Air preheat has a significant effect on the NO_x emissions while firing SRC."

5. Clark et al.¹ summarize the results, in part, of their investigation of synfuel liquid utilization in a utility gas turbine as:

- "Several fuel additives with the potential to reduce hot corrosion were investigated. Barium salts provided substantial corrosion protection.
- "Thermal-barrier coating can also protect turbine hot components from corrosion.
- "Several coatings provided substantially longer turbine life than a fully stabilized zirconia coating that was developed for use with clean fuels.
- "A study was conducted to estimate the potential cooling-hole plugging in the combustion environment of coal-derived fuels. It was concluded that plugging is a strong function of contaminant levels, plugging can be expected at low cooling flow rates, and plugging can be nearly eliminated at very high coolant flow rates."

6. Cabal et al.⁸ made the following conclusions based upon their work on the utilization of coal-derived fuels in a combustion turbine engine:

- "H-Coal distillate and SRC recycle liquid can be readily forwarded and atomized.
- "In general, the combustion wall temperature is higher when burning coal liquids than for base No. 2 petroleum fuel. Combustor wall temperature decreases with increasing hydrogen content of hydroprocessed coal liquid. The most severely hydroprocessed H-Coal distillate showed no increase in wall temperature over the base petroleum fuel. On the other extreme, the raw SRC recycle solvent (7.4 wt % hydrogen) caused burn-out of the combustor can in less than two hours.
- " NO_x emissions were 30% higher for the raw SRC recycle solvent (0.62 wt % fuel bound nitrogen). Increasing hydroprocessing severity decreased the fuel bound nitrogen content and produced fuels with NO_x emissions equivalent to the petroleum fuel.

*Heavy fractions of SRC may not be compatible with petroleum based fuels.

- "Coke formation on the fuel nozzle used in the combustor is a major concern with raw and mildly hydroprocessed coal liquids. These deposits ranged from massive for the raw SRC recycle solvent to nil for the most severely hydroprocessed SRC and H-Coal liquids. The severity of deposits in full scale combustors may be less due to higher flow rates.
- "Unburned hydrocarbon emissions are acceptable, increasing slightly with increasing fuel hydrogen. CO emissions are acceptable.
- "Smoke emissions were low for H-Coal liquids. Reliable smoke numbers could not be obtained for the SRC recycle solvent due to possible soot and coke formation in the sample line.
- "Flame temperatures were not significantly different for any of the fuels tested as determined by optical pyrometry."

7. Quinlan and Siegmund³ summarize the combustion properties of coal liquids from the Exxon donor solvent (EDS) process as follows:

"In summary, the EDS process produces a liquid product state from coal which can provide both a gasoline blend stock and several possible fuel oil. Potential applications for these fuel oils include utility boiler fuel, stationary turbine fuel and domestic heating oil. Product characterization studies for Illinois coal liquids have shown that the properties of heavy and middle distillate blends generally compare well with ASTM specifications for conventional petroleum fuels. Combustion studies have shown that the coal liquids are operable in conventional fire-tube boilers and domestic oil burners. Smoke and particulate emissions from combustion of EDS Illinois coal liquids are generally lower than conventional petroleum fuels. The fuel nitrogen levels in raw products are higher than experienced with conventional petroleum fuel oils. Combustion modifications or techniques like ammonia injection will likely be required to reduce nitrogen oxide emissions. Product hydrotreating to reduce fuel nitrogen content is also being considered. In order to meet future emission regulations on SO_x, product hydrotreating may be necessary for products from high sulfur coals like Illinois."

8. Longwell⁹ in his analysis of the utilization of synfuel liquids as transportation fuels, noted that "Much more research is needed in the chemistry of soot formation and burnout, and the mechanics of reactive flows involving high molecular weight liquids and vapors and soot, for the complex systems of practical interest."

The end results of the various synfuel liquid combustion demonstration tests are that, although these fuels with varying degrees of hydrogenation can be burned in numerous combustion devices, certain problems exist. The major

problems noted were NO_x emissions, plugging and fouling, and corrosion of hot spots. These tests were, of necessity, short-term tests of specific fuel samples and did not evaluate long-term effects of a broad range of synfuel liquids on the combustor or environment, nor were the tests developed to optimize combustor component designs. However, they did help identify problem areas and the need for an integrated research program.

VI. LITERATURE SURVEY OF DROPLET AND SPRAY COMBUSTION

Over the years, there have been a number of reviews of the "state of the art" of spray combustion. Wise and Agoston (1958)¹⁰ were early reviewers. Williams (1973)¹¹ reviewed the subject, emphasizing the application and diagnostic characterization of spray combustion. Williams again (1976)¹² published a review dealing with the special topics of heavy-oil spray combustion. One of the latest and most complete reviews of droplet and spray combustion was published by Faeth (1977)¹³ in which he presented considerable material on various devices and models of spray combustion. A review by Krishna (1978)¹⁴ covers recent activities in developing and applying numerical modeling to combustors and furnaces. A summary of each of these reviews follows with emphasis on those aspects of spray combustion that relate to the utilization of synfuel liquids:

1. The survey of liquid-droplet burning by Wise and Agoston¹⁰ gave an excellent account of the theoretical and experimental predictions of the combustion and burning rate of spherical liquid droplets. The effects of convection on the burning rate, based on boundary-layer theory and experimental data, have also been incorporated into the model to account for the enhanced burning rate due to convection. These corrections are expressed in terms of Reynolds and Schmidt numbers. Experimental results pertaining to preignition, ignition, and combustion of various liquid fuels, including gasoline and lighter diesel oil, are also presented.

Although the burning characteristics of gasoline and light diesel oil are found to follow a predicted linear relationship between the square of the drop diameter and time, this relationship was not observed with a heavy oil. The survey also gave a brief account of the effects of pressure, gas-phase composition, liquid-phase composition, and ambient gas flow on the burning rate and flame configuration. Of particular interest is the explosive phenomenon associated with the combustion of larger kerosene droplets (600-700 μ m), which were found to exhibit momentary brightening of the flame just before extinction. The phenomenon was also found to occur in preoxidized tetralin droplets in 30% heavy oil.

2. A comprehensive review of the combustion of droplets of liquid fuels was published by Williams (1973).¹¹ The paper presents information on the ignition and combustion of stationary and moving droplets in an oxidizing atmosphere, and the effect of high pressure on monopropellant combustion. A brief account of the application of single droplet combustion to a wide variety

of spray burners was also presented. Major theoretical developments occurring during the period since the Wise and Agoston¹⁰ review include classification and identification of the effects of finite chemical kinetics on flame structure, burning rate, and the ignition. Other developments deal with transient combustion characteristics owing to variations in droplet temperature, liquid-phase cracking in a heavy oil, influence of the wake field on flame configuration and burning rate, the burning rate of arrays of suspended droplets, flame propagation through one-dimensional systems (though no quantitative assessment concerning the effects of droplet interaction on the burning rate coefficient have been identified), multicomponent liquid fuel droplet combustion, the significance of liquid-phase cracking, irregular burning behavior, and the effect of thermal decomposition on the formation of carbonaceous residues and smoke.

3. An excellent survey of the combustion of oil was published by Williams¹² in an article entitled "Fundamentals of Oil Combustion" in 1976. Comparative discussions pertaining to combustion of lighter liquid fuels and heavy fuel oil have been held to elucidate the complex processes of heavy oil combustion characterized by disruptive boiling, droplet swelling, liquid cracking, thermal decomposition and the formation of smoke and cenosphere.

Experimental studies of heavy fuel-oil droplet combustion reveal that the combustion of such droplets is unsteady and irregular because of fractional distillation and liquid-phase cracking. Williams¹² notes that few analytical studies have been made and that most of the information on heavy-oil combustion processes has been obtained in experimental studies.

There has been considerable research interest in the formation of particulates by liquid-phase cracking of heavy fuel oil and thermal decomposition of hydrocarbons. These processes are considered to depend on the aromatic content of the heavy fuel oil with high asphaltene content. Although little is known about the mechanism of the production of carbonaceous particles, the formation of carbonaceous residues may be minimized by finer atomization or water emulsification of the heavy fuel oil.

The fuel-bound nitrogen in heavy fuel oil has been identified as a major source for NO_x pollutant in spray combustion. Relatively high efficiency in the conversion of fuel nitrogen to NO_x has been observed, viz., 100% for a low-level nitrogen content of 0.1% and 50% for a higher nitrogen content of 0.5%.

4. A review of the status of droplet and liquid combustion has been published by Faeth¹³ in 1977. The paper presents an excellent exposition on spray-combustion systems, various

elemental processes in spray combustion, and a comprehensive review and assessment of spray models and their application to various spray-combustor systems. Current spray models, including a correlation model, drop ballistics model, one-dimensional model, stirred-reactor model, locally homogeneous flow model, and laminar two-phase flow model, are discussed with detailed accounts of modeling criteria, methodology, and the results obtained with each method.

The correlation model provides empirical techniques to determine combustion properties and emission characteristics as functions of basic combustion data and relevant spray parameters, such as evaporation and fuel-air mixing. All the spray models, other than the correlation model, adopt an analytical approach which accounts for specific issues in the spray-combustion process (e.g., statistical aspects of droplet size distributions) to assess the effects of turbulent two-phase interactions on ignition and burning characteristics, such as length of spray flame, structure of the combustion zone, combustion efficiency, pollutant-emission characteristics, and the nature of laminar flame propagation.

Faeth¹³ discussed the general usefulness of the Equivalent Homogeneous Flow Model, which treats the spray-jet flame as a gas-jet flame with the same momentum and stoichiometry. This improved homogeneous model, which accounts for the turbulent transport processes developed by Khalil and Whitelaw,¹⁵ is identified as being an effective model for the overall assessment of combustion performance and emission characteristics of sprays containing droplets of smaller Sauter mean diameter i.e., $<45\text{ }\mu\text{m}$. Because this model is far less complicated than two-phase multidimensional flow models and has good predictive capability, the model merits further development, particularly in two directions: (1) clarification of the limitations of the model, and (2) identification of the optimal turbulent flow model.

The paper also gave a comprehensive assessment of the scope and potential of two-phase models, current working models, and numerical techniques, with specific references to the Particle-Source-In-Cell (PSIC) method. Areas of relevant research are also identified. Emphasis is placed on the need to improve gas-droplet interaction, and to gain information on multicomponent characteristics, drop-ignition criteria, and envelope flame stabilization. Further work on turbulent flow, verification of higher order closure in turbulent-flow theory, and effects of droplets on turbulent-flow characteristics are identified as areas needing more research efforts.

Faeth notes the limitations of dilute and nondilute spray theories and points out the lack of attention given to the development of nondilute spray theory and to experimentation.

5. "A Review of Furnace Modeling" by Krishna¹⁴ presents a qualitative survey of stirred-reactor models and fundamental models, with emphasis on the latter. A stirred-reactor model basically assumes that the characteristic times of the mixing process are small compared with reaction times. A more sophisticated stirred-reactor model adopts the concept of different degrees of mixing to accommodate finite mixing rates. A fundamental model, which accounts for detailed fluid dynamic processes, coupled with chemical kinetics, and heat and mass transfer, has been developed to predict the combustion environment and pollutant emission in the presence of flow recirculation, swirling, and radiation. A number of furnace models, including the Combustion Engineering Model, the ASH (Axi-Symmetric Heater) Model, developed by Harwell and Imperial Colleges, the United Technology Research Model, the Patankar and Spalding Model, and two other models for turbo-combustors are presently available. All the models except the Combustion Engineering Model use the Navier-Stokes equation, together with a turbulence model. Finite-difference schemes, together with various algorithms, are adopted to predict the combustion fields, which are described by a set of nonlinear elliptic partial differential equations. The predicted combustion fields are reported to be in qualitative agreement with limited experimental measurements.

These models are also applicable to liquid-spray and pulverized combustion in furnaces. However, limited experimental data are available for comparison with model results. Krishna¹⁴ concluded that further research efforts should be devoted to understanding (1) turbulence and turbulence-kinetic interactions in the presence of flow recirculation and swirling, (2) mechanisms of spray formations, and droplet interaction with turbulent flow fields, (3) combustion kinetics, pollutant formation, and radiation, (4) improvement of numerical methods, and (5) complex furnace geometry.

VII. RECENT DEVELOPMENTS RELATED TO SYNFUEL LIQUID SPRAY COMBUSTION

Information presented in this section on current research activities related to synfuel liquid combustion was obtained through a literature search for the period of 1977-1979, computer identification of sponsored research projects (1977-1978), and personal communication with scientists and engineers in these fields. Literature review of research programs linked with the demonstration of synfuel utilization in industrial furnaces and turbo-combustors, as described in the previous section, indicated that the potential for broader synfuel-liquid utilization is economically and environmentally sound, although a systematic experimental program for a prolonged period will be required to identify and resolve technical difficulties, some of which are identified in Section V.

Spray-combustion research efforts related to combustion characterization are now being assisted by the progress made in advanced combustion diagnostics including laser anemometry, laser interferometry, and laser diffraction techniques, which have been used in the measurement of velocity and size of droplets, and in spray spectra characterization. The diagnostic techniques, together with other sophisticated data-acquisition systems, paved the way to instrumentation and experimental validation of spray-flame configurations, spray-jet and flame structures, identification and quantification of major pollutants emitted by heavy oils, residual oil, and synfuel liquids.

Progress has also been made in understanding the collective interactions of droplets in practical sprays. Spray modular modeling such as the group combustion model and the droplet array model, has provided a theoretical base for the prediction of spray combustion and emission characteristics of typical combustors wherein the single-droplet combustion theory appears to be involved. The development of a realistic spray-flame model by using the existing single-droplet theory and group combustion theory, together with appropriate turbulent flow and chemical kinetics modeling, seems feasible; such a model could be extended to encompass spray combustion of synfuel liquids, provided that appropriate information pertaining to the multicomponent fuel characteristics of synfuel can be included in the modeling. There have been impressive research activities related to the assessment of pollutant emission from synfuel combustion. Data obtained in laboratory experiments are reproducible and can be used to develop practical correlations between NO_x and soot emissions and the fuel blend characteristics, together with combustion conditions.

Fundamental and semi-empirical kinetic mechanisms of hydrocarbon combustion are being developed and expanded under a current DOE contract at Princeton. The objectives of this work are to determine mechanistic oxidation routes for hydrocarbons, including aromatic compounds, derived from shale and coal, and to develop and validate simplified (global) reaction-rate and mathematical models for these hydrocarbons. Also included in this research is the study of reaction schemes and particulate (soot) production. Considerable background work by Dryer,^{16,17} Dryer and Glassman,¹⁸ and others¹⁹⁻²¹ is supportive in this effort. It is beyond the scope of this report to review the status of kinetic work. Because of the special nature of kinetic work, such a review should be considered for the future.

Analytical modeling capabilities emphasizing simplified modular models for the prediction of fuel effects on combustion characteristics are currently being studied as an extension of work by Blazowski *et al.*^{22,23} An example of these effects is the increased flame luminosity and exhaust smoke emission due to decreased hydrogen content of fuels. This development work is focusing on a stirred-reactor concept to characterize fuel effects on combustion phenomena.

Selected examples of sponsored research on spray combustion have been obtained through the ANL computer literature search facilities and EPRI publications. (The list of these sample research projects is presented in Appendix A.) The list identifies researchers, together with their affiliation, as well as the titles of the research projects and their sponsors.

Interviews and communications with selected research workers in areas related to spray combustion have been made to identify needed areas of research in synfuel spray combustion. A list of the people interviewed and a summary of their comments are presented in Appendixes B and C.

VIII. SYNUEL LIQUID COMBUSTION PROBLEMS

Improved understanding of the mechanisms that govern the combustion of liquid fuel sprays in practical combustion devices is currently of fundamental importance. Unfortunately, fuel spray combustion is a complex process, involving simultaneous heat, mass, and momentum transfer, and chemical reactions that are influenced by fuel type, ambient gas composition, temperature and pressure, droplet size distribution, and the relative velocity between the droplet and the surrounding gas. All of these factors are, in turn, influenced to varying degrees by the initial interaction of the air stream with the fuel spray, which affects the breakup of the liquid fuel sheets and subsequent droplet motion.

In considering the problems of utilization of synfuel liquids in turbines, boilers, and furnaces, this report will consider the problems in the same order as the steps in the combustion process--starting with fuel enhancement, then injection and atomization, preignition phenomena, ignition, combustion, combustion-chamber considerations, and, finally, pollutant formation. For each step, this report will consider the pertinent physical and chemical parameters, modeling and diagnostic techniques, and specific design problems as they relate to the spray combustion of synfuel liquids. Figure 1 presents a stylized concept of a typical spray combustor.

1. Fuel Enhancement

Muzio and Arand⁴ have shown that minute quantities of proprietary manganese-based additives are beneficial in reducing NO_x formation from fuel-bound nitrogen. Sangiovanni²⁴ has noted that as little as a one-percent change in the aromatic content of synfuel liquids can significantly affect ignition delay times. He has also noted that lighter fractions in the fuel (#2 fuel oil) lead to microexplosions of fuel droplets. This suggests that fuel tailoring may be beneficial to the combustion process. Fengier²⁵ suggests that the addition of barium salts to hydrocarbon fuels effectively inhibits soot formation. Birchley and Riley²⁶ have suggested a model to explain in part the greater combustion efficiency that is claimed for the combustion of emulsified fuels.

● There is need to know the extent to which the parameters in synfuel liquid ignition, combustion, and pollutant formation may be affected by fuel additives and/or fuel modifications. Work in this area will help in the optimization of combustor design and in establishing minimum hydroprocessing requirements for synfuel liquids.

Fig. 1. Stylized Spray Combustor

2. Injection, Plugging, and Corrosion Problems

Sullivan et al.²⁷ have reported plugging problems in preliminary combustion tests of synfuel liquids. Clark et al.¹ and Cabal et al.⁸ note that trace-metal contaminants have caused hot corrosion in gas turbine hot spots which would lead to extensive downtime for repairs.

● An experimental program is needed to establish limits and corrective procedures necessary to counteract injector plugging and corrosion before synfuel liquids can be efficiently utilized.

3. Prevaporization

Faeth¹³ notes that premixed combustion is currently being examined as a way of reducing NO_x formation in steady combustion systems. In a prevaporizing system, the fuel is injected into a heated air stream. Ideally, the drops are fully evaporated before reaching the flame, which is stabilized by a flame holder.

● There is a need to know which alternative fuels can be prevaporized and to establish prevaporization limitations for synfuel liquids. It is anticipated that lower-volatility coal liquids can have problems with flashback and preignition if prevaporization were employed to produce homogeneous gas combustion.

4. Injector Characteristics

The designer can greatly influence the combustion process by varying the design of the injector. Many different types of injectors are currently being used. These include twin-fluid injectors with either internal or external mixing, full or hollow-cone spray structures, swirl or tangential impinging jets, and the use of plain or pintle nozzles.

● A testing program is desired to determine optimum injection characteristics and their relationship to the use of synfuel liquids in new designs or in retrofit programs.

5. Atomization Characterization

The distributions of droplet sizes and velocities are required in the analysis of combustion sprays. This specification is complicated by the fact that spray formation involves the breakup of the primary jet, secondary droplet breakup, and collision between drops, yielding an evolving distribution of drop sizes and velocities. Droplet formation near atmospheric conditions occurs by the mechanism of aerodynamic disintegration. New theories reported by Dombrowski et al.²⁸ propose that ion-induced perforative disintegration of liquid sheets occur in the presence of hot flame fronts. For approximate analysis of vaporization and combustion, the Sauter mean diameter is often

used. This is the ratio of volume to surface area that is equivalent to a monodispersed spray. Numerous distribution functions of spray spectra have been proposed to characterize droplet size distributions. However, none of these are based upon physical parameters, and the investigator is obliged to choose the one that provides the best correlation with experimental data. Numerous correlations have been suggested between specific injector types and various average and median drop-size parameters. Although these are specific for the injector designs, designs are variable and quantitative work requires characterization of the particular injector under consideration.

- The use of synfuel liquids will require quantitative work on specific injector types to characterize synfuel liquid sprays.

6. Droplet Diagnostics

Traditionally, droplet size and velocities have been measured by impaction using magnesium oxide-coated slides or high-speed photography with double-spark illumination. These techniques are useful in single-drop or very diffuse spray investigations, but are of limited use in studies of dense combusting sprays. In recent years the advent of laser interferometry, laser droplet velocimetry, and holographic techniques have greatly expanded diagnostic techniques of spray combustion. Unfortunately, these latter techniques are relatively expensive and unwieldy, requiring image-processing equipment and computer-analyzing capabilities.

- Modification and improvement of diagnostic techniques for measuring synfuel liquid droplet size and velocities are required to effectively analyze spray combustion processes for this fuel.

7. Preignition Vaporization

While radiation effects on the vaporization rates of low-boiling-point liquid fuels are considered to be negligible, the greater opacity of synfuel liquids will result in greater radiation effects. Furthermore, vaporization rates of synfuel liquids are dependent upon the compositions of these multi-component mixtures with their differing contents of volatiles.

- Studies are needed to characterize preignition vaporization rates of synfuel liquids that will be used in spray combustion processes.

8. Recirculation and Slip

Very little is known about the recirculation effects of air and hot combustion gases on heat and mass transfer.¹³ Information is lacking on the three-dimensional effects near the injector, flow stabilizing, transient effects, the impact of various model parameters on the results, and the injector characteristics in hot recirculating flows.

Chigier et al.²⁹ have shown that significant differences in the velocities for various drop sizes within combustion sprays exist. The drop size of heavy oils tends to be larger, even after heating to 100°C.³⁰ Slip

occurs and refers to distortion of the droplet. The existence of aspherical droplets may affect various modeling assumptions. Slip will affect burning rate and flame configuration.

Industrial furnaces and gas turbines commonly use recirculation zones to control flame geometry, and increase flame stability and combustion intensity. These zones are produced by bluff bodies positioned in the air stream. At present, little quantitative information is available regarding recirculation zones, although it is recognized that "matching" of aerodynamics to fuel spray is important.²⁹

- The effect of slip needs more consideration to establish the limitations of assuming local homogeneity. Experimental work and modeling are needed to characterize synfuel liquid recirculation effects.

9. Preignition Phenomena

Williams¹² has noted that while the combustion of light fuel oils proceeds in a more or less orderly fashion, the combustion of heavy oils occurs in a more complex way. Due to radiation effects and the presence of high-boiling-point components within heavy fuel droplets, extensive swelling and disruptive boiling, followed by microexplosions within the droplets, can be expected. Except for the early stages of combustion when the more volatile components are being evaporated, the combustion of synfuel liquids can be described only by non-steady state analysis. Due to the difficulties of handling both fractional distillation and liquid-phase cracking mathematically, very few analytical studies have been made and most of the information about medium and heavy fuel oils has been derived from experimental studies.

- There is need for experimental work to identify the effects of the preignition phenomena, such as droplet swelling, disruptive boiling, microexplosions, fractional distillation, and liquid-phase cracking, on the modeling assumptions required to characterize synfuel liquid spray combustion.

10. Ignition and Combustion

Thermal ignition of a liquid fuel droplet involves preheating, vaporization, formation of a flammable mixture, and a rapid exothermic gas-phase reaction. Differences in characteristics of broad-cut boiling-point, multicomponent synfuel liquid fuel will alter the rate of formation of the flammable mixture, major exothermic reaction processes, and ignition. The fractional distillation/differential vaporization of synfuel liquid droplets will impose time-dependent characteristics on ignition and combustion processes.

The classical case of droplet burning is one that involves a volatile liquid fuel burning in a surrounding oxidizing atmosphere. The droplet evaporates and acts as a source of fuel vapor which burns with the surrounding oxidant as a diffusion flame around the droplet. The behavior of medium and heavy fuel oil droplets is markedly different from that of lighter fuel oils.¹² Figure 2 shows a comparison of the progress of ignition and combustion of a volatile pure-liquid droplet to that of the ignition and combustion of a residual-oil fuel droplet.

Fig. 2. Plot of Diameter Squared versus Time for Pure Volatile Droplets and Multicomponent Residual-Oil Fuel droplet.

It has been shown that droplet evaporation and ignition are influenced by neighboring drops, and that combustion of droplet arrays should be considered. Theories have recently been proposed to explain droplet interaction effects. Sangiovanni and Keston³¹ have shown that droplet interaction can have significant effects on ignition delay times. Chiu et al.³²⁻³⁴ and Labowski and Rosner³⁵ have proposed a "Group Combustion Theory" which is a new model of burning sprays that admits the effect of strong collective behavior of droplets on spray flame configurations. This theory indicates that a single droplet is not likely to occur in a typical turbocombustor or industrial furnace. Instead, groups of droplets are likely to burn with a large envelope flame which may be either located in the gas phase surrounding the spray jet or stabilized in the boundary of the spray jet. Such spray-group envelope flames have been observed in a number of independent experimental studies, with good reproducibility.^{29,36,37} The identification of a prospective combustion mode is based on the magnitude of a group combustion number, which is defined as the ratio of the rate of heat transfer from the envelope flame to the convective heat transfer rate of a reference flow. When the group combustion number exceeds a critical value, a group envelope flame occurs; otherwise, a single droplet or multidroplet combustion mode occurs within the spray jet. Such a difference should be accounted for in performance analyses and burner design. The effects of combustion chambers on the ignition and combustion phenomena should also be considered.

Edelman provided a thorough survey in 1977 on the status of laminar and turbulent gas dynamics in combustors which included a review of heterogeneous effects and combustion aspects in relation to gas dynamic processes in flames.³⁸

● There is a need for experimental and theoretical analysis of ignition and combustion characteristics of synfuel liquid droplets. The effects of fractional distillation/differential vaporization, swelling, disruptive

boiling, and droplet interaction need to be characterized. Realistic group combustion models need to be developed for various regions in the combustion zone. The models should be supplemented with accurate descriptions of turbulence-spray interaction, characteristics of spray spectra, synfuel liquid properties, and chemical kinetics of gas- and liquid-phase reactions, such as gas- and liquid-phase pyrolysis and chemical kinetics of polycyclic organic matter, as well as mechanisms of soot formation. Combustion parameters should be identified to facilitate optimal burner design and burner retrofit.

11 Combustion Chamber Components

The spray combustion of synfuel liquids tends to form more soot because of their lower hydrogen-to-carbon ratio. The impingement and interaction of synfuel liquid droplets and synfuel liquid combustion products will affect wall corrosion and erosion, overall heat-transfer characteristics, and the reliability, maintainability, and safety of combustion chamber components.

- Minimum-scale boiler model tests are needed to characterize the effects of synfuel liquid spray combustion on combustion chamber and heat-exchanger components. Also minimum-scale experimental model tests will be required to characterize similar effects on stationary gas turbines.

12. Emissions from Synfuel Liquid Combustion

Demonstration combustion tests of synfuel liquids have shown that emission problems may be expected. Due to the lower hydrogen-to-carbon ratio, higher aromatic content, more bound nitrogen, and presence of higher-boiling-point liquids in synfuel liquids, their spray combustion will entail problems of emissions of particulates and NO_x . It is believed that SO_x and CO emissions will not be significantly different from emissions encountered in spray combustion of conventional petroleum products.

- There is a need to characterize the nature and quantity of particulate and gaseous emissions from spray combustion of synfuel liquids. Trace-metal contaminants and their effect on hot corrosion need to be studied. Particular attention needs to be given to the area of possible carcinogenic emissions from the combustion of synfuel liquids.

IX. CONCLUSIONS

While spray combustion is being used in a more or less effective manner as a means of converting chemical energy to heat energy, the design and construction of combustion systems has traditionally proceeded in an empirical fashion. Designs of new systems have been based on trial and error variations of older systems. Considerable effort has been devoted to the development of a quantitative understanding of certain primary combustion phenomena, with the goal of developing a rational approach to the design of combustion systems. Although considerable progress has been made, numerous gaps still exist in our knowledge of spray-combustion phenomena. These gaps must be closed before truly optimal spray-combustion systems can be developed.

Anticipated large-scale development and utilization of synfuel liquids as a partial solution to the nation's energy dilemma will necessitate closing the gaps in our knowledge of spray-combustion phenomena.

The physical and chemical characteristics of synfuel liquids are significantly different from those of the liquid fuels that are normally burned today. Combustion system designers will no longer be able to design for a narrow range of liquid fuel properties, but will instead have to accommodate a broad range of fuel characteristics.

For the effective use of synfuel liquids in spray combustion as these fuels become available as alternative fuel sources to supplement domestic petroleum supplies, the following technological needs have been identified.*

1. Development of a technology data bank and analytical combustor models for industry based on the application of research to aid in the analysis, further research development, design scale-up, and operation of boilers and furnaces with alternate fuels.
2. Development of integrated programs within which experimental studies can be made in environments which are controlled and yet representative of those encountered in current and future combustors. Program goals will be to obtain realistic design criteria through integrated analytical modeling-experimental programs for both retrofit of existing stationary combustion devices and the development of new combustor concepts.
3. Continuous development and application of theoretical models of both the global and detailed types. Particular emphasis should be placed on development of "Group Combustion," "Droplet Arrays," and statistical models.
4. Further exploitation of stirred-reactor models and experiments for the characterization of the behavior of recirculation zones with intense backmixing. Information is lacking on three-dimensional effects near the injector, transient effects, the impact of various model parameters on the results, and injector characteristics in hot recirculating flows.
5. Quantitative understanding of primary atomization and secondary shattering of droplets in turbulent flow with the goal of characterizing spray spectra.
6. Chemical kinetic studies on the oxidation and pyrolysis of aromatics, particularly aromatics containing nitrogen, to characterize pollutant formation and emission problems.

*No intent has been made to present the technological needs in any order of priority.

7. Investigation of turbulent flames in configurations which allow systematic progression, starting with premixed and/or prevaporized system to diffusion flames with direct liquid injections, with the goal being the establishment of a coherent theory of spray combustion.
8. Studies of the coupling of turbulence and chemical kinetics.
9. Specific research on the formation of soot, NO_x , and polycyclic organic matter.
10. Studies of the effects of fuel additives and emulsions on ignition and combustion characteristics, and the formation of pollutants.
11. Studies of the corrosion and erosion effects of synfuel liquid spray combustion on combustors.
12. Development of improved instrumentation diagnostics with emphasis on real time temperature measurements in a system with laser diagnostics.
13. Attempts should be made to simplify modeling by use of global chemical kinetics and modular model concepts.

In conclusion, the authors wish to quote Dr. Hartwell F. Calcote, President, Aerochem Research Laboratories in his summary statement at the Project SQUID Workshop on Alternative Fuels Technology.³⁹ Dr. Calcote said, "There is a real need for a U.S. combustion program--a real program with mileposts and with practical objectives at given times." It is hoped that this report will be helpful in introducing investigatory milestones pertaining to spray combustion and in identifying some of the attributes that such a program might have.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the support and encouragement of this project by the Pittsburgh Energy Technology Center. Thanks are also given to the many researchers listed in Appendix B for their help and comments.

REFERENCES

1. J. S. Clark et al., Gas Turbine Critical Research and Advanced Technology Support Project: FY 1980, Annual Report COE/NASA 2593-79/6, NASA TM-79139.
2. Aron, Scaling Up Coal Liquids, EPRI Journal (September 6-13, 1978).
3. C. W. Quinlan and C. W. Siegmund, Combustion Properties of Coal Liquids from the Exxon Donor Solvent Process, Amer. Chem. Soc. Symposium on Combustion of Coal and Synthetic Fuels, Anaheim, CA, 23(1), 139 (March 1978).
4. L. J. Muzio and J. K. Arand, Small Scale Evaluation of the Combustion and Emission Characteristics of SRC Oil, Amer. Chem. Soc. Symposium on Combustion of Coal and Synthetic Fuels, Anaheim, CA, 23(1), 140-150 (March 1978).
5. J. B. Jordan, G. M. Kimber, and A. Williams, Ignition of Droplets of Liquid Fuels Solvent Extracted from Coal, Fuel 56, 417-421 (1976).
6. B. F. Piper, S. Hersh, and W. Nazimowitz, Combustion Demonstration of SRC-II Fuel Oil in a Tangentially Fired Boiler, KVB Inc., Report Summary FP-1029, May 1979.
7. J. E. Haebig and B. E. Davis, Preliminary Small-Scale Combustion Test of Coal Liquids", Environ. Sci. Technol, 10 (3), 243-247 (1976).
8. A. V. Cabal et al., Utilization of Coal-Derived Liquid Fuels in a Combustion Turbine Engine, Amer. Chem. Soc. Combustion of Coal and Synthetic Fuels Symposium, Anaheim, CA, 23(1), 119-138 (March 1978).
9. J. P. Longwell, Synthetic Fuels and Combustion, Sixteenth International Symposium on Combustion, 1-15 (1976).
10. H. Wise and G. A. Agoston Burning of a Liquid Droplet, Adv. Chem. Sci. 20, 116-135 (1958).
11. A. Williams, Combustion of Droplets of Liquid Fuels: A Review, Combust. Flame, 21, 1-31 (1973).
12. A. Williams, Fundamentals of Oil Combustion, Prog. Energy Combustion Sci., 2, 167-179 (1976).
13. G. M. Faeth, Current Status of Droplet and Liquid Combustion, Prog. Energy Combustion Sci., 3, 191-224 (1977).

14. C. R. Krishna, A Review of Furnace Modeling, BNL 5088, Brookhaven National Laboratory (June 1978).
15. E. E. Khalil and J. H. Whitelaw, Aerodynamic and Thermodynamic Characteristics of Kerosene-Spray Fluid, Sixteenth International Symposium on Combustion, 569-574 (1978).
16. F. L. Dryer, The High Temperature Oxidation of CO and CH₄, Fourteenth International Symposium on Combustion, The Combustion Institute, Pittsburgh, PA, 987 (1973).
17. F. L. Dryer, High Temperature Oxidation of Carbon Monoxide and Methane in a Turbulent Flow Reactor, Princeton University Ph.D. Thesis, Report No. 1034T (1972).
18. F. L. Dryer and I. Glassman, Combustion Chemistry of Chain Hydrocarbons, Princeton University Aerospace and Mechanical Sciences Report No. 1350, Workshop on Alternate Hydrocarbon Fuels for Engines: Combustion and Chemical Kinetics, Columbia, Maryland, Sept. 7-9, 1977.
19. F. L. Dryer and C. K. Westbrook, Detailed Models of Hydrocarbon Combustion, Proceedings of the Department of Energy, Division of Power Systems, Workshop on Modeling of Combustion in Practical Systems, Los Angeles, CA, January 4-8, 1978.
20. K. P. Schug, R. J. Santoro, F. L. Dryer, and I. Glassman, An Investigation of the Pyrolysis and Oxidation of Ethylene in a Turbulent Flow Reactor, Presented at the 1978 Spring Meeting Western States Section of the Combustion Institute, Boulder, CO (1978).
21. C. K. Westbrook, J. Creighton, C. Lund, and F. L. Dryer, A Numerical Model of Chemical Kinetics of Combustion in a Turbulent Flow Reactor, J. Phys. Chem. 81, 2542 (1977).
22. W. S. Blazowski, Dependence of Soot Production on Fuel Blend Characteristics and Combustion Conditions, ASME 79-GT-155, Gas Turbine Conference and Solar Energy Conference, March 12-15, 1979.
23. W. S. Blazowski, R. B. Edelman, and P. T. Harsha, Fundamental Characterization of Alternate Fuel Effects in Continuous Combustion Systems, Exxon Research and Engineering Company, Summary Technical Progress Report, August 15, 1977-August 14, 1978 C0011543-12 (September 11, 1978).
24. J. Sangiovanni, Investigation of Combustion Characteristics of Fuel Droplet Arrays, United Technologies Research Center, Final Report, September 1979.
25. A. Fengier, Effect of Metal Additives on the Amount of Soot Emitted by Premixed Hydrocarbon Flames, Adv. Chem. Ser. 166, 178-189 (1978).
26. J. C. Birchley and N. Riley, Transient Evaporation and Combustion of a Combustion Water-Oil Droplet, Combust. Flame 29, 145-165 (1977).

27. R. F. Sullivan, C. E. Rudy, and H. C. Chen, Refining and Upgrading of Synfuels from Coal and Oil Shales by Advanced Catalytic Processes, Quarterly Report April-June 1978, FE2315-28, Chevron Research Corp.
28. N. Dombrowski, W. Horne, and A. Williams, The Formation and Combustion of Iso-octane Spray in Hot Gases, Combust. Sci. Technol. 9, 247-254 (1974).
29. N. A. Chigier, C. G. McCreath, and R. W. Makepeace, Dynamics of Droplet in Burning and Isothermal Kerosene Spars, Combust. Flame 23, 11-16 (1974).
30. L. A. Kennedy, Ed., Turbulent Combustion, Progr. Astro. & Aeronaut. 58 (1978).
31. J. J. Sangiovanni and A. S. Keston, Effect of Droplet Interaction on Ignition in Monodisperse Droplet Streams, 16th Int. Symp. on Combustion, 577-591 (1978).
32. H. H. Chiu et al., Spray Group Combustion, AIAA 16th Aerospace Sciences Meeting, Huntsville, AL, January 1978.
33. H. H. Chiu and T. M. Liu, Group Combustion of Liquid Droplets, Combust. Sci. Technol. 17, 127-142 (1977).
34. T. Suzuki and H. H. Chiu, Multidroplet Combustion of Liquid Propellants, Proc. Ninth Int. Symp. on Space Technology and Science, 145-154 (1971).
35. M. Labowski and D. E. Rosner, Group Combustion of Droplets in Fuel Clouds. I. Quasi-Steady Predictions, Proc. Symp. on Eval/Comb. of Fuel Droplets, 63-79 (1978).
36. C. G. McCreath and N. A. Chigier, Liquid-Spray Burning in the Wake of a Stabilizer Disc, Fourteenth International Symposium on Combustion, 1355-1363 (1973).
37. Y. Onuma and M. Ogasawara, Studies on the Structure of Spray Combustion Flame, Fifteenth International Symposium on Combustion, pp. 453-465 (1977).
38. R. B. Edelman and P. T. Harsha, Laminar and Turbulent Gas Dynamics In Combustors - Current Status, Prog. Energy Combust. Sci., 4(1), 1-62 (1978).
39. C. T. Bowman and J. Birkeland, Alternative Hydrocarbon Fuels: Combustion and Chemical Kinetics, Prog. Astronaut. Aeronaut. 62 (1977).

APPENDIX A

SELECTED EXAMPLES OF SPONSORED COMBUSTION RESEARCH

1978 - 1979

<u>Researcher</u> (Organization)	<u>Research Title</u> (sponsoring agency)
1. W. Bartok (Exxon)	Application of combustion modification to control pollutant emission for power generation combustion system (EPA)
2. D. R. Bartz (KVB Engineering, Inc.)	Application of combustion modification technology to industrial combustion equipment (EPA)
3. H. Bernstein (Hittman Assoc.)	Assessment of environmental implication of Project Independence (Unspecified)
4. W. S. Blazowski (Exxon)	Fundamental characteristics of alternative fuel effects in continuous combustion systems (DOE)
5. U. Bonne, <u>et al.</u> (Honeywell)	Combustion research on increasing thermal efficiency, reducing pollutant generation and improving flame sensing and ignition methods (Honeywell, Consolidated Gas, SC Gas Co., NBS, EPA, Amer. Gas Assoc.)
6. A. V. Cabal, <u>et al.</u> (Mobil), (Westinghouse), (EPRI)	Utilization of coal-derived liquid fuels in a combustion turbine engine (EPRI)
7. S. Carmi and K. A. Kline (Wayne State U.)	Rheology of coal-oil slurries as it relates to stability, spray formation, and combustion (DOE)
8. H. H. Chiu and E. J. Croke (U. of IL), (ANL)	Spray group combustion (DOE)
9. E. M. Dickson and R. M. Rodden (SRI)	Impact of synthetic liquid fuels development (EPA)
10. F. Dryer and I. Glassman (Princeton U.)	Fundamental combustion studies of emulsified fuels (DOE) Fundamental and semi-global kinetic mechanisms of hydrocarbon combustion (DOE)
11. G. W. Dykema (Aerospace Corp.)	Analysis of NO _x control in stationary sources (EPA)

APPENDIX A (contd)

<u>Researcher (Organization)</u>	<u>Research Title (sponsoring agency)</u>
12. C. Foster (Gen'l Motors)	Demonstration of potential in plant-sized environment for using emulsified fuel (DOE)
13. S. R. Gollahalli (Oklahoma U.)	Combustion of water-oil emulsions (Oklahoma U.)
14. C. Hartman (Accurex Corp.)	Pilot-Scale evaluation of advanced combustion control technology for fossil and waste (EPA)
15. M. P. Heep, J. E. Cichanowicz, and M. L. Lobell (Energy and Environmental Research Corp.)	Effects of fuel properties and atomization parameters on NO _x control for heavy liquid fuel-fired package boilers (EPA)
16. J. B. Howard (MIT)	Combustion research on coal nitrogen and particulate organic matter (EPA)
17. J. B. Howard and A. F. Sarofim (MIT)	Study of Soot Burnout in Flames (NSF)
18. R. W. Hurn (DOE)	Automotive testing of synthetic fuels (DOE)
19. H. G. Johnson (Suntech)	Fossil fuels research (DOD, EPA, DOE)
20. J. Keck and J. B. Heywood (MIT)	Mechanism of NO, CO, and HC formation in combustion (EPA)
21. W. S. Lanier (EPA)	Evaluation of fundamental combustion phenomena (EPA)
22. W. S. Lanier and B. Demetriades (Ind. Environ. Res. Lab.)	Direct measurement of combustion factor effects on secondary particulate formation (EPA)
23. C. K. Law (Northwestern U.)	Combustion studies of coal-in-oil droplets (NSF)
24. A. Levy (Battelle Columbus Lab.)	Staged combustion for NO _x control and enhanced SO ₃ emissions (EPA)
25. J. B. Longwell, A. F. Sarofim, J. Beer, and J. B. Howard (MIT)	Health Effects of Fossil Fuel Utilization (HEW)

APPENDIX A (contd)

<u>Researcher (Organization)</u>	<u>Research Title (sponsoring agency)</u>
26. G. B. Martin and W. Butts (EPA)	Characterization of emission and combustion performance of alternate fuels (EPA)
27. H. B. Mason (Acurex Corp.)	Environmental assessment of stationary source NO _x control technologies (EPA)
28. B. J. Mathews (TRW, Inc.)	Emissions assessment of conventional combustion systems (EPA)
29. F. O. Mixon (Research Triangle Inst.)	Pollutants from synthetic fuels production (EPA)
30. R. D. Moranie (So. Counties Co.)	Burning test of solvent refined coal (DOE)
31. L. J. Muzio and J. K. Ranad (KVB, Inc.)	Small-scale evaluation of the combustion and emission characteristics of SRC-II oil (Unspecified)
32. P. Nettesheim (National Inst. of Environ. Health Sci.)	Carcinogenesis of fossil fuel-related combustion products (National Inst. of Environ. Health Sci.)
33. W. H. Nuridr (Rockwell Inter. Corp.)	Fuel decomposition and flame reactions in conversion of fuel nitrogen to NO _x (EPA)
34. H. E. Nuttal, Jr. (New Mexico U.)	Experimental investigation of oil shale pyrolysis and combustion phenomena (Occidental Research Group)
35. C. Peranok (ANL)	Early and late effects of energy-related pollutants on experimental animals - evaluation of the tumorigenic enhancing potential in liver of polycyclic aromatic hydrocarbons (DOE)
36. D. E. Polymeropoulos (Rutgers U.)	Spark ignition of liquid fuel sprays (NSF)
37. R. M. Price, C. E. Smith, and B. S. Hinton (Pratt & Whitney)	Low NO _x combustion development for stationary gas turbine engines (DOE)
38. C. W. Quinlan and C. W. Siegmund (Exxon)	Combustion properties of coal liquids from Exxon donor solvent process (Exxon)
39. J. Rife, J. B. Heywood, and J. P. Longwell (MIT)	Modeling Diesel Engine Particulates (GM)

APPENDIX A (contd)

<u>Researcher (Organization)</u>	<u>Research Title (sponsoring agency)</u>
40. J. J. Sangiovanni (UTRC)	Investigation of combustion characteristics of fuel droplet arrays (DOE)
41. W. A. Sirignano (Princeton U.)	Combustion of multicomponent liquid fuel droplets (DOE)
42. W. A. Sirignano (Princeton U.)	Ignition and flame propagation in sprays (Army Research Office)
43. W. A. Sirignano and H. S. Homan (Princeton U.)	Vaporization and combustion of multi-component liquid fuel droplets (NSF)
44. A. F. Sarofim and J. P. Longwell (MIT)	Control of NO _x emissions from combustion of fuels derived from shale and coal (DOE)
45. A. G. Sharkey, Jr. (DOE)	Hazardous and other undesirable elements and compounds in supplementary gaseous and liquid fuels from coal (DOE)
46. R. E. Thomas (KVB Eng., Inc.)	Application of combustion modification techniques to control pollutant emissions from industrial boilers (EPA)
47. M. F. Tyndall (Catalytic, Inc.)	Environmental assessment/system analysis utilizing residual oil (EPA)
48. T. J. Tyson (Energy and Environ. Res. Corp.)	Fundamental combustion research applied to pollution control (EPA)
49. A. Vranos (UTRC)	Combustion investigation of heavy oil sprays (DOE)
50. J. H. Wasser (EPA)	Emission control technology for high pressure combustion systems (EPA)
51. C. R. Wolfe (Westinghouse)	Hazardous substance in residual oil (EPA)
52. V. Zakkay and W. Brenner (New York U.)	Experimental study of the effect of fuel vaporization on combustion efficiency (DOE)

APPENDIX A (contd)

<u>Organization*</u>	<u>Research Title (sponsoring agency)</u>
1. Acurex Corp.	Combustion catalysts for coal derived liquids with high-bound nitrogen (EPRI)
2. Air Preheater Co.	Effects of NH ₃ -based NO _x control on air preheaters (EPRI)
3. Babcock & Wilcox	Combustion tests of SRC-II with dual register burner (EPRI)
4. Consolidated Edison	Combustion demonstration of SRC-II coal liquid (EPRI)
5. Consolidated Edison	Particulate and trace element emission characteristics on oil-fired utility boilers (EPRI)
6. KVB, Inc.	Combustion demonstration of SRC-II coal liquid (EPRI)
7. KVB, Inc.	Evaluation of alternative low-NO _x furnace designs (EPRI)
8. Meteorology Research, Inc.	Trace element removal characteristics of particulate control devices (EPRI)
9. Mobil	Exploratory studies in catalytic coal liquefaction (EPRI)
10. Stearns-Roger, Inc.	Operational aspects of ammonia-based NO _x control technology (EPRI)
11. Stone and Webster Eng.	Conversion of oil-fired boilers for use of coal-derived liquid fuels (EPRI)
12. Univ. Of Wyoming	Wyodak solvent refined coal upgrading system (EPRI)
13. Westinghouse	Baseline data on utilization of low-grade fuels in gas turbine applications (EPRI)

*Investigators unidentified

APPENDIX B

LIST OF RESEARCH WORKERS CONTACTED

The following is a list of researchers contacted during the period of this review. Their comments are summarized and listed in Appendix C.

<u>Researcher</u>	<u>Affiliation</u>
1. Blazowski, W. S.	Exxon Research and Engineering Co., Corporate Research, Technology Feasibility Center, Linden, New Jersey
2. Bonne, U.	Honeywell Corporate Research Center, Bloomington, Minnesota
3. Bracco, F. V.	Princeton University, Princeton, New Jersey
4. Brzustowski, T. A.	University of Waterloo, Waterloo, Ontario
5. Driscoll, J. M.	The University of Michigan, Ann Arbor, Michigan
6. Dryer, F. L.	Princeton University, Princeton, New Jersey
7. Edelman, R. B.	Science Applications, Inc., Woodland Hills, California
8. Faeth, G. M.	The Pennsylvania State University, University Park, Pennsylvania
9. Glassman, I.	Princeton University, Princeton, New Jersey
10. Gollahalli, S. R.	The University of Oklahoma, Norman, Oklahoma
11. Law, C. K.	Northwestern University, Evanston, Illinois
12. Liu, T. M.	General Electric Co., Schenectady, New York
13. Mellor, A. M.	Purdue University, West LaFayette, Indiana
14. Penner, S. S.	University of California at San Diego, LaJolla, California
15. Rosner, D. E.	Yale University, New Haven, Connecticut

APPENDIX B (contd)

<u>Researcher</u>	<u>Affiliation</u>
16. Sangiovanni, J. J.	United Technology Research Center, East Hartford, Connecticut
17. Sarofim, A. F.	Massachusetts Institute of Technology, Cambridge, Massachusetts
18. Sichel, M.	The University of Michigan, Ann Arbor, Michigan
19. Sirignano, W. A.	Princeton University, Princeton, New Jersey
20. Williams, F. A.	University of California at San Diego, LaJolla, California
21. Zakkay, V.	New York University, New York, New York

APPENDIX C

SAMPLE COMMENTS OF INTERVIEWEES

The following is a summary of selected comments by individuals contacted during the period of this review. These comments are in response to a request as to what problem areas or research needs exist in the areas of synfuel liquid spray combustion. These comments are not listed in order of priority but are simply a reflection of various communications with the individuals listed in Appendix B.

- Comprehensive data base and physical-chemical characterization of synfuel for burner component design, performance analysis and emission control would be useful for modeling and design.
- Need for data of fuel-bound nitrogen; its oxidation and the control of NO_x .
- Fuel stability at high preheating temperature and its effect on the atomization needs to be understood.
- Nozzle fouling and clogging at high average temperature near the injector head is a problem area.
- Comparative assessments are needed of coal derived liquids, shale oil, SRC-II, and EDS; and to establish guidelines for an incremental refining of synfuel liquids.
- Carcinogenicity of pollutants and their control technology should be investigated.
- Establish a comprehensive technological approach for the combustion of very heavy liquid by-products.
- Pre vaporization, vaporization, and ignition characteristics of synfuel liquid droplet and droplet clouds should be studied.
- Technique of mixing alcohol in a solution of other petroleum liquids as means of secondary atomization should be investigated.
- Need development of technology for spray combustion of slurry fuel, coke particle slurry, SRC refined oil.
- Development of a spray combustion modulating technique for periodic or partial loading should be considered.
- Need for technology development and specific combustion diagnostic technique, as required in the course of complete spray characterization.
- Mechanisms of soot formation, and soot distribution and impact on radiative environment in furnace needs consideration.

APPENDIX C (contd)

- Adaptability of twin-flow and air-blast injectors for synfuel spray combustors needs to be confirmed.
- Need for accurate specifications of initial and boundary conditions for spray modeling.
- Collective intercoupling of droplet-droplet gas-phase interactions and their effects on the spray flame structure, burning, and emission characteristics require investigation.
- We need to study variations of combustion modes in a spray and their effects on pyrolysis, cracking, thermal decomposition and soot formation.
- We should identify major spray parameters, and make evaluations of spray operations.
- We really don't know the mechanisms and effects of interactions of droplets with turbulent flow.
- Investigations of vaporization, ignition, pyrolysis, thermal decomposition, liquid phase reaction, and fractional distillation of multicomponent synfuel droplet are needed.
- Techniques of fuel tailoring for synfuel should be identified.
- Effects of convection and temperature of environment on soot formation and extinction need to be investigated.
- There is a need for modeling of synfuel spray combustion and model ranking.
- Kinetics of liquid-phase reaction is a real problem.
- Emphasis should be placed on atomization of liquid, liquid-phase pyrolysis, soot formation, and staged combustion to control pollutants.
- Comprehensive emission control strategies for NO_x , particulates, and soot formation in gas turbine combustors should be developed.
- We need identification of optimal spray combustion for industrial furnaces, turbocombustors, and diesel engines.
- Techniques of burning and retrofitting are required for synfuel utilization.
- Mechanism of spray flame propagation and stabilization of synfuel sprays are areas of concern.
- Effects of disruptive boiling and droplet shattering on spray spectra characteristics must be considered.
- There is a need for a synfuel data base and dissemination of technical information pertinent to synfuel burner design and operation for users.

APPENDIX C (contd)

- There is need for the development of spray submodeling and global modeling.
- Effects of turbulent correlation associated with temperature, velocity, and concentration fluctuations on combustion require investigation.
- Nondestructive two-phase turbulent combustion diagnostics is an important research need.
- Correlations of synfuel properties with evaporation and combustion characteristics, such as volatility, ignition, blow-off, quenching, burning rate, and emissions of various pollutants, are essential for spray burner design.
- Application of synthetic fuel in advanced combustion systems with high burner efficiency is needed to implement fuel conservation objectives.
- Determinations of rheological properties of alternate liquid fuels under various conditions is required for the design of injectors.
- Determinations of atomization characteristics at different pressures, temperatures, and injector configurations for optional spray injection are of practical value in injector design.
- Analytical models and experimental studies related to turbulent spray in an enclosure are essential for the evaluation of burner performance and the establishment of design guides.
- Details of the chemical kinetics of oxidation, pyrolysis, and the mechanism of soot formation need to be understood to develop viable emission control strategies.
- Economic studies relative to synfuel refinement are needed for broader commercialization of alternate liquid fuels.
- Studies are needed to assess the effects of transient heating processes on ignition characteristics and flame propagation of large, high-boiling-point synfuel liquid droplets.
- Interactions between gas phase and multi-droplet systems need to be investigated.
- Various explanations for envelope flames surrounding a combusting spray require further investigation to delineate relevant mechanisms which can be used in advanced turbulence interaction models
- There is a need for modeling and experiments which quantify the effects of turbulence/radiation interactions in spray combustion.
- Advanced techniques of generating well-controlled arrays of droplet stream are required for the experimental research of droplet arrays.

APPENDIX C (contd)

- Development of proper conservation equations for two-phase flow and the correct identification of characteristics of equations, together with proper selection of initial and boundary conditions are of basic importance in spray analysis.
- Detailed descriptions and comparative studies linked with the sizes of droplets and turbulent eddies are essential for spray modeling.
- There is a need to develop an array of diagnostic techniques to determine detailed transient processes of droplets in synfuel spray combustors.
- Application of diagnostic techniques developed in nuclear technology would be useful for the measurement and the characterization of droplets.
- Experimental and theoretical work related to the determination of the formation of soot and NO_x emission in two-phase flow is essential for understanding the emission characteristics of burners and furnaces.
- Quantitative data are needed on the formation of soot and the presence of polynuclear aromatic compounds resulting from the combustion of alternative fuels. Lack of understanding of aerodynamic effects seriously flaw almost all of the available data.
- Progress is being made on understanding fuel nitrogen conversion; however, data are needed on interaction of nitrogen species (radicals and compounds) with hydrocarbon species and with soot.
- There is a need to develop synfuel spray injection and atomization processes which would avoid preignition, nozzle clogging, and particle depositions.
- Practical means of avoiding fuel breakdown due to fuel instability is needed for synfuel injection processes.
- Erosion effects of particulates and soots on gas turbine blades require further investigation.