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REVIEW OF ALTERNATIVE FUELS DATA BASES

FINAL REPORT

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ABSTRACT

Based on an analysis of the interaction of fuel physical and chemical properties with combustion characteristics and indicators, a ranking of the importance of various fuel properties with respect to the combustion process has been established. This ranking has been used to define a suite of specific experiments whose objective is the development of an alternative fuels design data base. Combustion characteristics and indicators examined include droplet and spray formation, droplet vaporization and burning, ignition and flame stabilization, flame temperature, laminar flame speed, combustion completion, soot emissions, NO_x and SO_x emissions, and the fuels' thermal and oxidative stability and fouling and corrosion characteristics. Key fuel property data is found to include composition, thermochemical data, chemical kinetic rate information, and certain physical properties.

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SUMMARY

Based on an analysis of the interaction of fuel physical and chemical properties with combustion characteristics and indicators, a ranking of the importance of various fuel properties with respect to the combustion process has been established. This ranking has then been used to define a suite of specific experiments which will lead to a comprehensive alternative fuels design data base. The specific combustion experiments are outlined in Table S1. These experiments encompass unit process investigations (plug flow and well-stirred reactor; flat flame and diffusion flame; droplet combustion and spray characterization), experiments designed to introduce in a simplified form the effects of combustion aerodynamics (well-stirred reactor/plug flow with distributed injection; spray vaporization and burning in a uniform flow), and experiments designed to provide data on the coupling of the mechanisms involved in turbulent flames within the context of a model of a realistic industrial burner flowfield. This suite of combustion experiments, and the associated analysis of the experimental results, would provide a comprehensive design data base for the use of alternative fuels in industrial burners. Table S1 includes the specific output from each class of experiment, the rationale for each experiment, and the fuel property data that is required to properly interpret the experimental results. Finally, since the interpretation of experimental combustion data requires the use of analytical techniques, as does the scaling of given experimental results to apply to conditions beyond those measured or at sizes different from those considered in the experiments, required analytical models for each type of experiment are indicated in the last column.

Fuel physical and thermodynamic property data are required to properly analyze and interpret the data from most of the experiments listed in Table S1. While some attempts have been made to collect and analyze available physical and chemical property data for alternative fuels, the available data base remains fragmentary and incomplete. For example, very little work has been done to critically analyze the available information from the standpoint of its utility to the burner designer, and data over a wide range of temperatures is generally not available. Thus, a major aspect of the initial phase of the suggested data

TABLE S1. Combustion Experiments for Alternative Fuels Effects Determination.

EXPERIMENT TYPE	EXPERIMENT OUTPUT	RATIONALE	FUEL PROPERTY DATA REQUIRED FOR INTERPRETATION	MODELS REQUIRED FOR INTERPRETATION/SCALING
1. PLUG FLOW REACTOR • GAS PHASE FUEL OR PREVAPORIZED; PREMIXED.	Species and temperature as function of time, inlet temperature, fuel/air ratio, pressure, heat loss. Ignition delay time. Intermediate species, NO_x, SO_x, soot. Combustion completion time.	Kinetics data; ignition data. Determine key intermediates, relationship between intermediates and NO_x, SO_x, soot. CO/HC emissions data.	Fuel composition. Fuel thermodynamic properties.	One-dimensional plug flow analysis. Finite-rate chemical kinetics formulation.
2. WELL-STIRRED REACTOR (a) GAS PHASE FUEL OR PREVAPORIZED, PREMIXED.	Species as function of residence time, inlet temperature, fuel/air ratio, pressure, heat loss. Emissions characteristics-NO_x, SO_x, soot. Blowout limits.	Kinetics data, emissions characterization, soot limits, combustion stability limits.	Fuel composition. Fuel thermodynamic properties.	Well-stirred reactor analysis. Finite-rate chemical kinetics formulation.
(b) LIQUID PHASE FUEL	As above, as function of spray quality.	Effect of liquid fuel properties on emissions, sooting, combustion stability.	As above, with liquid fuel properties, spray characteristics.	Multiphase well-stirred reactor analysis. Finite-rate chemical kinetics formulation. Droplet vaporization/burning model. Residence-time distribution function model.
3. LAMINAR & TURBULENT FLAMES • GAS PHASE FUEL OR PREMIXED. (a) FLAT FLAME, PREMIXED.	Flame speed, species and temperature histories. Intermediate species, NO_x, SO_x, soot, as function of inlet fuel/air ratio, temperature, heat loss.	Reactivity determination, relative to fuel type, fuel/air ratio, temperature. Data for kinetics model development. Interaction of chemical kinetics with laminar and turbulent flowfield, transport properties. Effects of transport property variation. Ignition/stabilization limits.	Fuel composition. Fuel thermodynamic properties. Gas-phase transport properties. Effective emissivities for gas phase, soot.	Laminar flat flame model, with effects of diffusion, chemical kinetics, variable transport properties. Radiation heat loss model.
(b) DIFFUSION FLAME • PARTIALLY PREMIXED AND PURE DIFFUSION.	As above.	As above.		Laminar bunsen flame model, parabolic steady-state and elliptic time-dependent, with effects of diffusion, chemical kinetics, radiation heat loss.
4. SINGLE DROPLET COMBUSTION (a) OPTICAL MEASUREMENTS.	Drop diameter as a function of time, ambient temperature, fuel type.	Burning rate coefficient and transfer number determination.	Fuel type.	Classical single drop model.
(b) DETAILED MEASUREMENTS.	As above, with detailed measure of species evolved in vaporization, burning of drop. Pyrolysis of droplet. Formation of cenospheres. Drop temperature as function of time.	As above. Investigate fuel pyrolysis, formation of cenospheres as function of fuel type, ambient environment. Data for detailed drop combustion model. Kinetics of fuel decomposition.	Fuel composition, thermodynamic properties, liquid-phase physical properties.	Detailed nonuniform temperature multicomponent fuel droplet combustion model. Finite-rate kinetics formulation.

TABLE S1. Combustion Experiments for Alternative Fuels Effects Determination (continued).

EXPERIMENT TYPE	EXPERIMENT OUTPUT	RATIONALE	FUEL PROPERTY DATA REQUIRED FOR INTERPRETATION	MODELS REQUIRED FOR INTERPRETATION/SCALING
5. COMBINED WSR/PLUG FLOW WITH DISTRIBUTED INJECTION (a) GAS PHASE FUEL OR PREVAPORIZED.	Exit species as function of residence time, inlet temperature, fuel/air ratio, primary/secondary air injection rate, heat exchange in plug flow.	Examine in controlled simulation effects of aerodynamics and staging in combustion process as a function of fuel type. Determine techniques for minimizing NO_x, SO_x, soot. Investigate quenching effects.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data.	Coupled well-stirred reactor/plug flow with distributed injection in plug flow. Finite-rate chemical kinetics.
(b) LIQUID PHASE FUEL	As above, as function of fuel liquid properties, fuel type.	As above. Examine effects of air preheat on combustion process for liquid fuels.	As above, with liquid fuel properties, spray characterization.	Multiphase well-stirred reactor/plug flow with distributed injection model. Finite-rate chemical kinetics, droplet combustion model.
6. SPRAY CHARACTERIZATION	Droplet size, distribution as function of injector type, fuel type, fuel temperature, pressure, primary and secondary air flow rate.	Determine influence of fuel properties on spray droplet size and droplet distribution function. Investigate interaction of spray injector, fuel type, and airflow velocity as affects drop size.	Fuel liquid-phase physical properties.	Spray formation analysis - numerical or semiempirical.
7. SPRAY VAPORIZATION/ BURNING - UNIFORM FLOW	Combustion characteristics - species profiles, SO_x, NO_x, soot; temperature as function of fuel spray quality, air temperature, heat transfer rates; simplified aerodynamics.	Determine overall effects of fuel properties on combustion processes in simplified model burner simulation. Investigate effects of air preheat, staging, for spray fuel injection.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data. Effective thermal emissivity. Fuel liquid properties. Spray characterization.	Spray transport/vaporization/burning analytical model. Coupled finite-rate chemistry; single droplet and spray burning models.
8. ALTERNATIVE FUELS COMBUSTION IN A MODEL BURNER (a) GAS PHASE FUEL OR PREVAPORIZED.	Combustion characteristics - species profiles, NO_x, SO_x, soot, temperature as function of fuel type, fuel/air ratio, air temperature, heat transfer rates, representative burner aerodynamics: large scale recirculation zones, swirl.	Determine overall effects of alternative fuels on combustion processes in aerodynamics representative of industrial burners.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data. Effective thermal emissivity.	Industrial burner combustion model: turbulent mixing, recirculation zones, swirl, coupled finite-rate chemistry.
(b) LIQUID PHASE FUEL	As above, with addition of spray quality as a parameter.	As above, with addition of spray injection representative of industrial liquid-fuel burners.	As above, with addition of: Fuel liquid properties. Spray characterization.	Multiphase industrial burner combustion model; add spray transport to above specification.

base development work is the compilation of the physical and thermodynamic properties of the fuel, as shown in Table S2. This work also includes compilation of fuel composition data, for with appropriate composition data it is possible to estimate fuel properties when measured properties are not available. These estimated fuel properties can then be used in the analysis of the combustion experiments listed in Table S1, and the results of this analysis will in turn indicate the sensitivity of the particular combustion process to the estimated property value. This iterative procedure will identify those fuel properties for which estimated values are insufficiently accurate, so that more accurate values can be obtained by direct experimental measurement.

The basic data generation phase of the suggested program includes stirred reactor and plug flow combustion experiments, single droplet combustion experiments, spray characterization experiments, and liquid properties data compilation work in addition to the composition, thermodynamic, and physical properties data compilations already discussed. These basic experiments would provide the data, including chemical kinetic and liquid burning rate information and spray droplet size and distribution, necessary to provide a preliminary assessment of the effects of alternative fuels on combustion processes in industrial burners.

To obtain more refined estimates of alternative fuels effects on the combustion processes in industrial burners, the work outlined under the preliminary properties effects determination phase in Table S2 would be carried out. Because a primary impact of alternate fuels with respect to industrial burners is anticipated to involve liquid fuel combustion processes, this phase incorporates multiphase well-stirred reactor experiments (which require the spray characterization work carried out in the preceding phase for their analysis and interpretation) and more detailed single droplet experiments. For both gas-phase alternative fuels and liquid fuels, the well-stirred reactor-plug flow experiments would provide an initial data base on the effects of aerodynamics, staging, inlet air heating, and other emissions control and efficiency improvement techniques. Thus, the overall output of this phase would be an evaluation of the effects of fuel properties on the combustion process in simplified systems that incorporate some of the important features of industrial

TABLE S 2

SUGGESTED DATA BASE DEVELOPMENT PLAN BY PHASE AND TASK

PHASE	TASKS	OUTPUT
Basic Data Generation	Thermodynamic properties compilation Fuel composition data compilation Chemical kinetic rate determination Single droplet combustion Fuel liquid properties compilation Spray characterization	Basic composition, physical and thermodynamic property data compilation Droplet burning rate data Drop size/distribution data
Preliminary Properties Effects Determination	Multiphase well-stirred reactor experiments Single droplet combustion (detailed data) Well-stirred reactor/plug flow experiments (gas phase and multiphase)	Effects of fuel properties on combustion process in simplified systems
Alternative Fuel Effects in Industrial Burners	Well-stirred reactor/ plug flow experiments (gas phase, multiphase) Spray vaporization and burning in uniform flow Model industrial burner experiments	Effects of fuel properties on the combustion process in realistic systems.

burners. Note that the properties data base, kinetics data base, and liquid-fuel combustion processes data base obtained in the initial phase of the suggested program are all necessary for the evaluation of the data obtained during this phase.

The third phase of the suggested program would be designed to provide a comprehensive quantification of the effects of the use of alternative fuels in flowfields representative of realistic industrial burners. This phase, as shown in Table S2, incorporates additional well-stirred reactor/plug flow reactor experiments, experimental investigations of spray combustion in a uniform flow, and experiments in a configuration designed to model the flowfield in an industrial burner. The output of this phase is a description of the effects of fuel properties on the combustion process in realistic systems. Taken together, the suggested program will thus provide a complete and comprehensive evaluation of the impact of the use of alternative fuels on industrial burner design.

Each of the experimental efforts outlined in Table S1 interacts to some extent with the other tasks of the suggested work, as is noted in the column entitled "fuel property data required for interpretation" in Table S1. Because of these interactions, certain of the tasks must follow the availability of data from other tasks, as is depicted on the phase/task/time interaction diagram, Fig. S1. As is shown in this figure, the initial tasks involve thermodynamic and physical properties data compilation and composition data compilation, as well as single-droplet burning rate determination. This is not meant to imply that no other work can be initiated until the properties data compilation is completed, since as outlined above, certain physical and chemical properties of the fuel may be estimated. Further, for many alternative fuels of interest an initial data base encompassing thermodynamic and physical properties, as well as single-droplet burning rate data, although fragmentary, already exists. Thus, although not shown explicitly in Fig. S1, assessment of the available data should be carried out concurrent with this phase of the suggested program. As the interactions shown on Fig. S1 suggest, there is a considerable degree of relationship between each of the tasks, but such a feedback is a basic requirement for any well-constructed program and would be anticipated in any program structured along the lines suggested in this report.

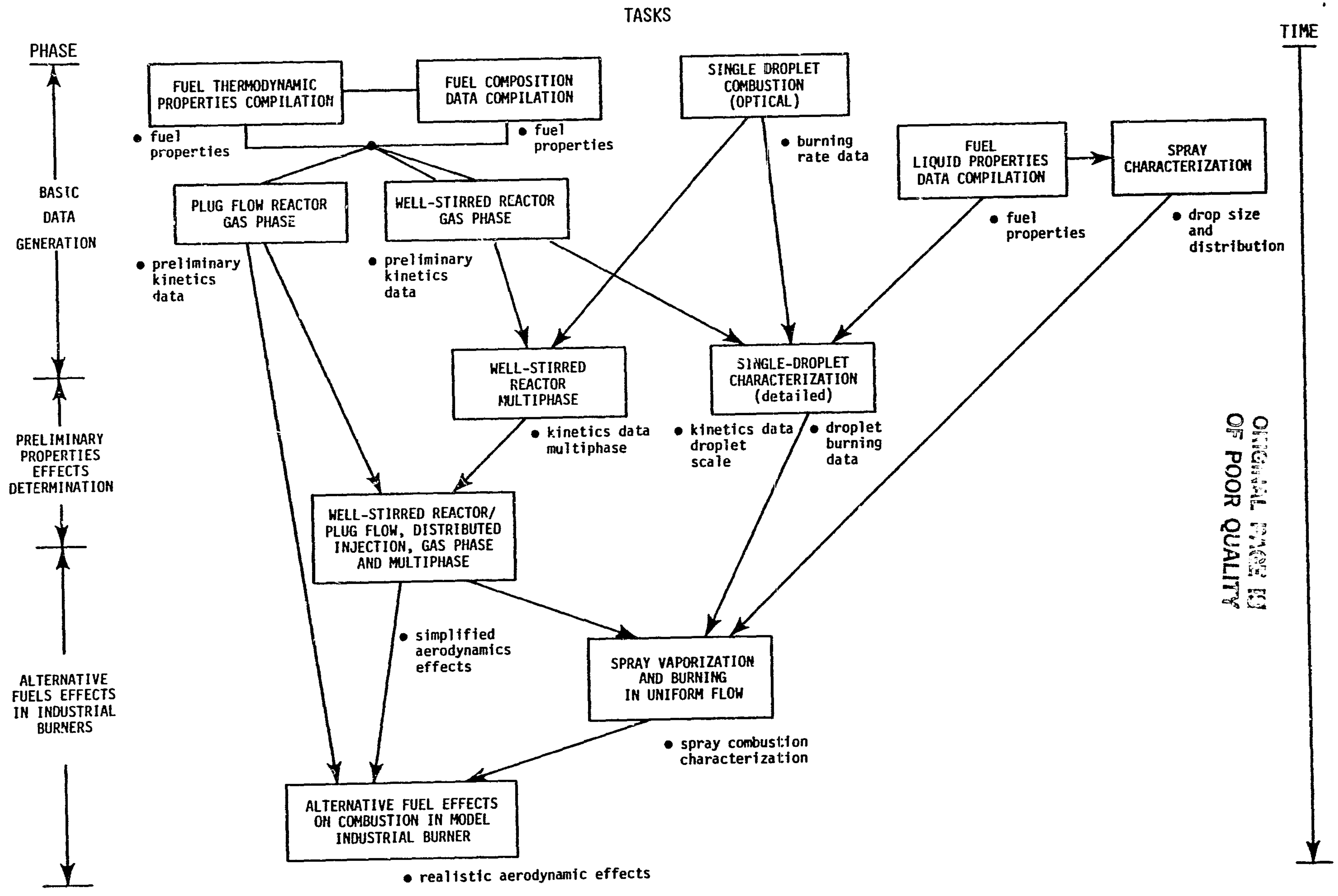

FIGURE S1. Phase-Task-Time Interaction Diagram - Alternative Fuels Effects Determination.

1. INTRODUCTION

The performance evaluation criteria used to select burners for industrial furnaces and boilers for specific applications include thermal efficiency, thermal output and flame shape, operational flexibility, fuel flexibility, and erosion, corrosion, and deposition characteristics (i.e., durability) when operated on specific fuels. In addition to these criteria, environmental constraints require the minimization (and near elimination) of NO_x, SO_x, and soot emissions; while these environmental constraints can, under some circumstances, be met by post-combustor exhaust gas cleanup, a more cost-effective and flexible approach is generally to achieve emissions reductions through burner design. Finally, in some applications industrial burners must operate over a wide range of fuel and air flows, i.e., have good turndown characteristics. This requirement can introduce problems with combustion instabilities in different portions of the burner operating envelope.

To meet a specific set of burner performance criteria, the industrial burner designer has available to him a number of design parameters. These include fuel selection, fuel injection method and location, control of the spray formation and vaporization process, control of primary and secondary air injection location and rate (combustion staging) and control of the burner configuration. The designer, as noted above, can also elect to control emissions characteristics through combustion process modifications. However, each of these parameters is typically constrained by operational aspects related to the intended burner application. Moreover, typical industrial burner design practice has involved the extrapolation of existing designs to new applications, rather than a "clean sheet of paper" design approach. This typical practice is driven by both a need to have maximum confidence in the suitability of the burner design for a given application, with minimal testing required and, often, the relatively small number of burners to be produced for a specific application.

An evolutionary approach has often been sufficient to meet burner design objectives because only incremental advances in performance characteristics were required and because the fuel to be used had been used in similar burners before. Current industrial burners have not had to cope with wide variations in fuel properties, particularly with respect to liquid and gaseous fuels. While some variation in liquid fuel properties is tolerable with respect to meeting the appropriate standards for the various grades of fuel oils, this variation does not have a strong impact on burner performance. Variations in gaseous fuel properties have also been small, at least as far as general natural gas supplies in the continental United States are concerned. However, this situation is expected to change in the relatively near future as synthetic liquid and gaseous fuels begin to take on greater importance in the overall fuel supply.

Synthetic liquid and gaseous fuels can be made to have properties similar to their petroleum-derived and natural gas counterparts, but the amount of refining necessary to do this can make the resulting product prohibitively expensive. If extensive refining can be avoided, more widespread use of synthetic fuels can be expected, but this requires that industrial burners be capable of meeting their performance and emissions requirements while using a broader range of fuels than has been attempted in the past. The difficulty facing the burner designer is that most synthetic (and many conventional) fuels have not been adequately characterized with respect to the physical and chemical properties of the fuels which affect the combustion process. Thus, the impact of broadened-specification fuels on combustor performance and emissions cannot be predicted, and appropriate design modifications cannot be developed.

The relationship between fuel properties and burner performance is outlined schematically in Figure 1. As the chart indicates, the chemical and physical properties of the fuel are intimately connected with the combustion mechanisms, comprised in turn of both chemical and physical elements. Thus, the overall dynamics of the combustion process are controlled by chemical and physical subprocesses (elements) which are directly relatable to fuel properties. The result of the complex series of interactions that takes place is the performance of the combustion process: this performance, when examined in the context of a specific burner, then defines the performance of a given industrial burner.

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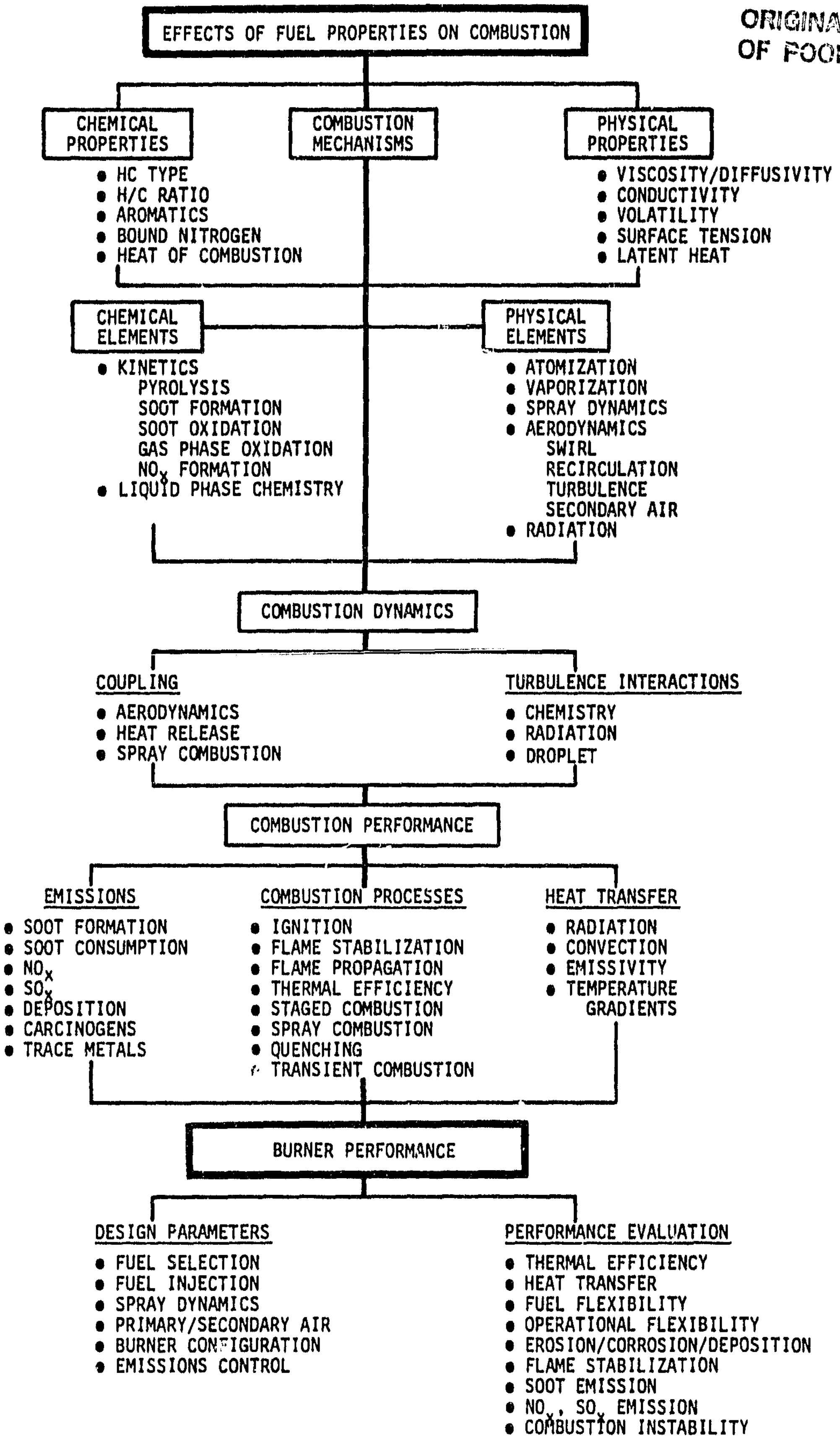

FIGURE 1. Relationship Between Fuel Properties and Burner Performance.

Figure 1 provides a schematic representation of the interactions between fuel properties and combustion characteristics in an industrial burner, but it does not define the relationships involved. This definition is a key issue in determining the requirements for an alternative fuels design data base. The objective of the work described in this report has been to define specific combustion characteristics which determine burner performance and their relationship to fuel properties. This leads in turn to an identification of areas in which further data on combustion characteristics and their relationship to fuel properties is required, and an identification of specific fuel properties necessary for a rational assessment of alternative fuels effects on burner design. The output of this work is thus a recommendation for experiments and analyses necessary to define and quantify the relationships between combustion characteristics and alternative fuel properties. This includes a prioritization of data requirements with those fuel properties which are most critical to the assessment of fuel effects on combustion given the highest priority. Following these recommendations, a plan for carrying out the work necessary to establish the required alternate fuel data bases is outlined. This includes the definition of fuel property table formats and questionnaires which can be used to establish in detail those data which are currently available.

2. TECHNICAL DISCUSSION

The interactions of a fuel's chemical and physical properties with characteristics of importance in determining burner performance are shown in Table 1. Note that this table includes chemical and physical property interactions with combustion characteristics (i.e., characteristics that affect burner performance from a combustion standpoint) as well as characteristics that apply to the usability of the fuel and the durability of the burner. Thus, thermal and oxidative stability are characteristics which impact fuel usability while fouling and corrosion affect burner durability. Both of these can influence the combustion process as well: thermal and oxidative stability through alterations of fuel physical properties and composition, and fouling and corrosion through unintentional alteration of burner flowfield characteristics.

The performance characteristics listed across the top of Table 1 are grouped into four general areas: liquid fuel combustion characteristics, which includes droplet and spray formation, droplet size, and droplet lifetime; gas phase combustion characteristics, which includes ignition phenomena, flame stability and flame temperature; measures of combustion completeness such as CO and HC (hydrocarbon) emissions, and pollutant emissions characteristics (NO_x, SO_x, and soot); and the usability and durability characteristics already mentioned. This division is of course arbitrary, since for a liquid fuel the formation, mixing, vaporization and burning of the spray profoundly influences the subsequent combustion process, while fuel characteristics, affected by thermal and oxidative stability, and combustor aerodynamics, affected by corrosion and fouling, both influence the spray combustion and gas phase ignition and flame stabilization processes. Nevertheless, dividing the performance characteristics in the manner done in Table 1 allows each group to be discussed together: the interactions within a group of characteristics are generally stronger than those between groups.

Liquid fuel combustion characteristics are those which relate to the preparation of the fuel-air mixture within the burner. Injection of the fuel into the burner produces a spray which involves a distribution of droplets, and this spray has characteristics which are determined by fuel properties, by the type and geometry of the fuel injection system, and by the interaction of the injected fuel with the air stream in the burner. During and subsequent to the

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TABLE 1. Chemical and Physical Property Interactions With Combustion Characteristics and Indicators.

GROUP	LIQUID FUEL COMBUSTION		BASIC COMBUSTION CHARACTERISTICS			CHEMICAL KINETICS			OPERATIONAL & DURABILITY			SUMMARY
COMBUSTION CHARACTERISTIC OR INDICATOR	DROPLET AND SPRAY FORMATION ①	DROPLET VAPORIZATION AND BURNING ①	IGNITION AND FLAME STABILIZATION ①	FLAME TEMPERATURE	LAMINAR FLAME SPEED	COMBUSTION COMPLETION ①	SOOT EMISSIONS ①	NO_x AND SO_x EMISSIONS ①	THERMAL AND OXIDATIVE STABILITY	FOULING ①	CORROSION ①	OVERALL RANKING
PHYSICAL PROPERTY	DEGREE OF PROPERTY INTERACTION: STRONG (S), MODERATE (M), WEAK (W), OR NEGLIGIBLE (N)											
HEAT OF COMBUSTION, ΔH_c (OR HEAT OF FORMATION, ΔH_f)	N	S	N	S	W	N	N	N	N	N	N	W
HEAT OF VAPORIZATION, ΔH_v	N	S	N or S	W	W	N	N	N	N	N	N	W
LIQUID DENSITY, ρ_L	M	S	N or S	N	N	N	N	N	N	N	N	W
LIQUID HEAT CAPACITY, C_{P_L}	N	M	N or S	N	N	N	N	N	N	N	N	W
LIQUID VISCOSITY, μ_L	S	W	N	N	N	N	N	N	N	N	N	W
SURFACE TENSION, σ	S	W	N	N	N	N	N	N	N	N	N	N
GAS HEAT CAPACITY, C_P	N	S	S	S	S	N	W	N	N	N	N	M
GAS VISCOSITY, μ	W	S	S	W	S	N	N	N	N	N	N	W
GAS THERMAL CONDUCTIVITY, k	N	S	M	N	S	N	N	N	N	N	N	M
GAS DIFFUSIVITY, D_{ij}	N	S	M	M	S	N	N	N	N	N	N	W
VOLATILITY	N	S	M	N	N	N	N	N	N	N	N	
CHEMICAL KINETIC RATES	N	M	S	W	S	S	S	S	N	N	N	M
COMPOSITION												
• ELEMENTAL ANALYSIS	N	M	M	S	S	S	S	S	M	M	S	S
• HYDROCARBON TYPE	N	M	S	S	S	S	S	W	S	M	S	S
• SPECIES ANALYSIS	N	M	S	S	S	S	S	S	S	S	S	S
• BOUND NITROGEN	N	N	N	N	N	N	N	S	W	W	W	W
• SULFUR	N	N	N	M	N	N	N	S	M	M	M	W
• SEDIMENT	N	M	M	M	N	N	W	W	S	S	M	W
• TRACE METALS, ACIDITY	N	N	N	M	N	W	W	W	S	S	S	M

① Indicates that this combustion characteristic or indicator is strongly influenced by the flowfield aerodynamics so that a careful analytical interpretation or an unambiguous experimental definition is required to provide useful quantitative data.

injection process, vaporization is taking place, and burning of the vapor-phase fuel can also occur in the environment surrounding the droplets. The vaporization and burning process clearly affects the droplet lifetime. Droplet lifetime, on the other hand, affects the burner length required to achieve complete combustion. Droplet lifetime also has an impact on flowfield aerodynamic features that are required to achieve complete combustion within a given burner length.

Vapor or gas phase combustion phenomena fall into two subgroups: those which are involved in ignition and flame stabilization, and those involved in combustion completion and production of the trace species and soot that constitute burner emissions characteristics. In the first category are ignition and flame stabilization phenomena (ignition delay time and blowout), flame temperature, and laminar flame speed. Ignition delay time, which is affected by the fuel's chemical kinetic rates, the ambient temperature, and local heat transfer phenomena, clearly sets a lower limit on the residence time required in a burner for combustion to occur. In general, this time is small, but the recirculation regions that serve as flameholding locations in a burner can also be small. For a sufficiently small recirculation region, or a sufficiently high rate of mixing of cold unburned gas into the recirculation region, residence time can fall below ignition delay time and blowout occurs. Thus, there is a close relationship between ignition delay and blowout (and flame stabilization phenomena in general), with flame stabilization involving the coupling of aerodynamic flow times and ignition delay times. Flame temperature is controlled by fuel thermodynamic properties and the initial temperature of the unburned mixture. It is a determinant of several aspects of burner performance, most importantly the heat output characteristics that can determine the suitability of a burner for a given application. Flame temperature is also important from the standpoint of NO_x and SO_x emissions characteristics, while soot formation and consumption in a flame can rapidly increase the flame luminosity, increasing radiant heat transfer from the flame while reducing the flame temperature. Finally, the laminar gas phase flame speed is an important characteristic by itself in some applications (e.g., low-speed burner flows where flashback phenomena may occur) as well as being a useful measure of the reactivity of a fuel. Since laminar flame speed is directly related to the chemical reaction rate, measurements of laminar flame speed for a variety of inlet flow fuel air ratios and temperatures can be used to estimate the chemical kinetic rate constants for a given fuel.

Chemical reaction time (as opposed to ignition delay time) is an important factor in determining the completeness of combustion and NO_x, SO_x, and soot emissions. If residence time is less than the reaction time, combustion will not be completed. This will reduce thermal NO_x emissions, since the fully-reacted temperature is never achieved, but increase CO and HC emissions, and have a deleterious effect on burner efficiency. Residence time is controlled primarily by the burner flowfield dynamics and mixing rate, while reaction time is a strong function of fuel-air ratio and temperature. In a flowing system, such as an industrial burner, the flowfield aerodynamics and the chemical kinetic phenomena that determine reaction time are clearly tightly coupled.

Usability and durability characteristics - thermal and oxidative stability, fouling, and corrosion - primarily involve the ability of the fuel to withstand long term storage and environmental extremes without major property changes, and the amount of ash and corrosive constituents in the fuel. Overall effect of these usability and durability characteristics on burner performance involve primarily the fuel management system and furnace and boiler components, but each of these characteristics can also affect combustion phenomena. For example, a fuel with poor thermal and oxidative stability characteristics will undergo changes which can affect the viscosity, surface tension, density, and composition of the liquid, thus affecting the droplet and spray formation process as well as subsequent droplet vaporization and burning. Similarly, fouling creates soot and ash buildups on burner and boiler/furnace components which can affect the burner aerodynamics, while corrosion induced by a fuel can alter fuel injection characteristics and, by eroding parts of a burner, burner aerodynamics. In extreme cases, fouling and corrosion processes can result in localized burnout of the burner lining and subsequent failure.

Arranged in different rows on the left-hand side of Table 1 are the various fuel physical properties which impact each of the burner performance characterization parameters discussed above. These include thermochemical parameters such as the heat of combustion (or heat of formation), which is a measure of the energy content of the fuel, and the heat of vaporization, which is a measure of the amount of energy required to vaporize fuel droplets. Physical properties such as the liquid density, viscosity and surface tension, gas phase viscosity and diffusivity, and thermophysical parameters such as the liquid heat capacity, vapor phase heat capacity, and vapor phase thermal connductivity impact all of the phases of the combustion process, controlling droplet vaporization and burning rates and vapor phase mixing rates directly, and chemical reaction rates indirectly through effects on mixture temperature.

For most alternative fuels (and many conventional fuels) determination of the thermochemical and physical properties is made difficult by the fact that the fuel is a mixture of different chemical species with different physical properties. Thus, for example, most fuels do not have a single boiling point at a given pressure, but fractionally distill - different constituents boil at different temperatures. Knowledge of the chemical composition of the fuel is thus highly important, but here the difficulty is the sheer number of different species that can be involved (and, for high molecular weight molecules, the number of isomers that are possible). Thus, a variety of composition determinations are required, including elemental analysis to determine the C-H-O-N ratios of a model fuel molecule, and analysis of the hydrocarbon type to determine aromaticity, as well as the breakdown of the fuel into aromatic and aliphatic components. Other determinations of importance include analyses of fuel-bound nitrogen, sulfer content, sediment (ash) content, and the content of trace metals and fuel acidity.

The body of Table 1 gives an indication of the degree of the property interaction between the thermochemical, thermophysical, and physical properties arranged on the left-hand side of Table 1, and the performance characterization parameters arranged across the top. These are listed as strong, moderate, weak, or negligible interaction, and this degree of interaction specification is what will be substantially used as an aid in establishing relative data priorities. This listing derives from a detailed study of each of the performance characterization parameters, as will be discussed in the remainder of this section. Following this discussion, the implications of the results summarized

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in Table 1 with respect to data needs for an alternative fuels design data base will be considered.

2.1 Liquid Fuel Combustion Characteristics

An example of the overall impact of fuel properties on combustion performance can be provided by the work carried out by Siminski [1]. This work, which was concerned with propulsion system applications, involved measurement of the combustion efficiency, η, for various fuels, in a simulated propulsion system combustor. While the conditions of these tests were different from those encountered in many (but not all) industrial burner applications, the results are of interest since they can be interpreted as providing evidence of the influence of fuel properties on overall burner performance.

A variety of fuels were studied by Siminski [1], and the data obtained showed a strong effect on η of inlet temperature at low inlet temperatures. The fuel was injected into the combustor in liquid form so that the vaporization rate of the fuel can be expected to have an impact on the overall combustor performance. Since η is related to the actual total temperature rise in the combustion process (ΔT_0 actual) divided by the ideal total temperature rise (ΔT_0 ideal), and this can, in turn, be related to the vapor fuel concentration α_v divided by the initial liquid fuel concentration, $\alpha_{F,0}$ which in turn is directly relatable to the fuel vaporization rate, a relation between η and vaporization rate can be devised:

$$\eta \propto \left(\frac{\Delta T_0 \text{ actual}}{\Delta T_0 \text{ ideal}}\right)^{1/2} \propto \left(\frac{\alpha_v}{\alpha_{F,0}}\right)^{1/2} \qquad (1)$$

and

$$\frac{\alpha_v}{\alpha_{F,0}} = 1 - \left(\frac{d}{d_0}\right)^3 \qquad (2)$$

where d_0 represents the initial droplet diameter and d the droplet diameter at subsequent time t, so

$$\eta = \left[1 - \frac{d}{d_0}^{3}\right]^{1/2} \qquad (3)$$

Since, using the classical "d^2" vaporization law

$$\frac{d^2}{{d_0}^2} = 1 - \frac{\lambda}{{d_0}^2}\,\frac{Nu}{2}\,t \qquad (4)$$

and the vaporization rate coefficient, λ, is a function of the gas-droplet temperature difference

$$\lambda = \frac{8k}{\rho_L C_p}\,\ell n\left[1 + \frac{C_p \Delta T}{L}\right] \qquad (5)$$

then the overall combustion efficiency can be seen to be a function of the gas-droplet temperature difference, ΔT.

In Eqs. 4 and 5, Nu is the Nusselt number, while k and Cp represent the vapor thermal conductivity and specific heat in the region surrounding the droplet, respectively; ρ_L is the liquid density and L is the fuel's heat of vaporization. This correlation was tested by computing vaporization rates as a function of the temperature difference between gas and droplet for two droplet sizes and two fuels, listed as fuels "A" and "B" in Table 2. As can be seen from Table 2, these fuels differ in properties such as molecular weight, viscosity at low temperature, and boiling point temperature. The solution for droplet diameter, d, is obtained through use of the "d^2" law coupled to one-dimensional statements of momentum and energy transport for the droplet exposed to a uniform gas-phase environment. Droplet diameter was computed at a time from injection corresponding approximately to the time required for the fuel to reach the flameholder in the combustor used by Siminski [1]. The agreement between the correlation and the data is striking for both fuels, as shown in Figure 2 and 3. The term C appearing in Fig. 2, is the coefficient providing the curve fit shown in the figure.) Since the droplet size in the apparatus used by Siminski was not known, a range of sizes was used; it might be expected that at similar conditions fuel "B" would form larger droplets than fuel "A" because of its higher viscosity. Note also from Fig. 2 that the agreement of the correlation for smaller droplets with the data at the higher fuel temperature is consistent with a reduction in drop size with fuel temperature increase (due to a fuel viscosity decrease); this is also seen for fuel "A", Fig. 3, for the lower ΔT (and therefore, higher fuel temperature) range.

TABLE 2

FUELS USED IN STUDY OF FUEL EFFECTS ON COMBUSTOR PERFORMANCE [1]

	Fuel A	Fuel B
Model Formula	$C_{10}H_{19}$	$C_{140}H_{184}$
Mean Molecular Weight	139.26	1867.01
Net Heat of Combustion (KCal/gm)	10.30	10.02
Heat of Formation (KCal/gm)	-0.41	0.13
Heat of Vaporization (KCal/gm)	0.30	0.34
Specific Gravity @ 293°K	0.818	1.042
Viscosity (CP) @ T	13.5 @ 239°K max	1876 @ 238°K
Boiling point °K	450	480
Freezing Point °K	227 max	233
Flash Point °K	333 min	389
Stoichiometric Air/Fuel Ratio	14.64	13.77
Specific Heat (estimated) (Cal/gm °K)	0.5	0.5

The fuel injection processes considered in the present work include droplet and spray formation, vaporization, and droplet burning. These processes have been the focus of a considerable amount of research effort, most of which

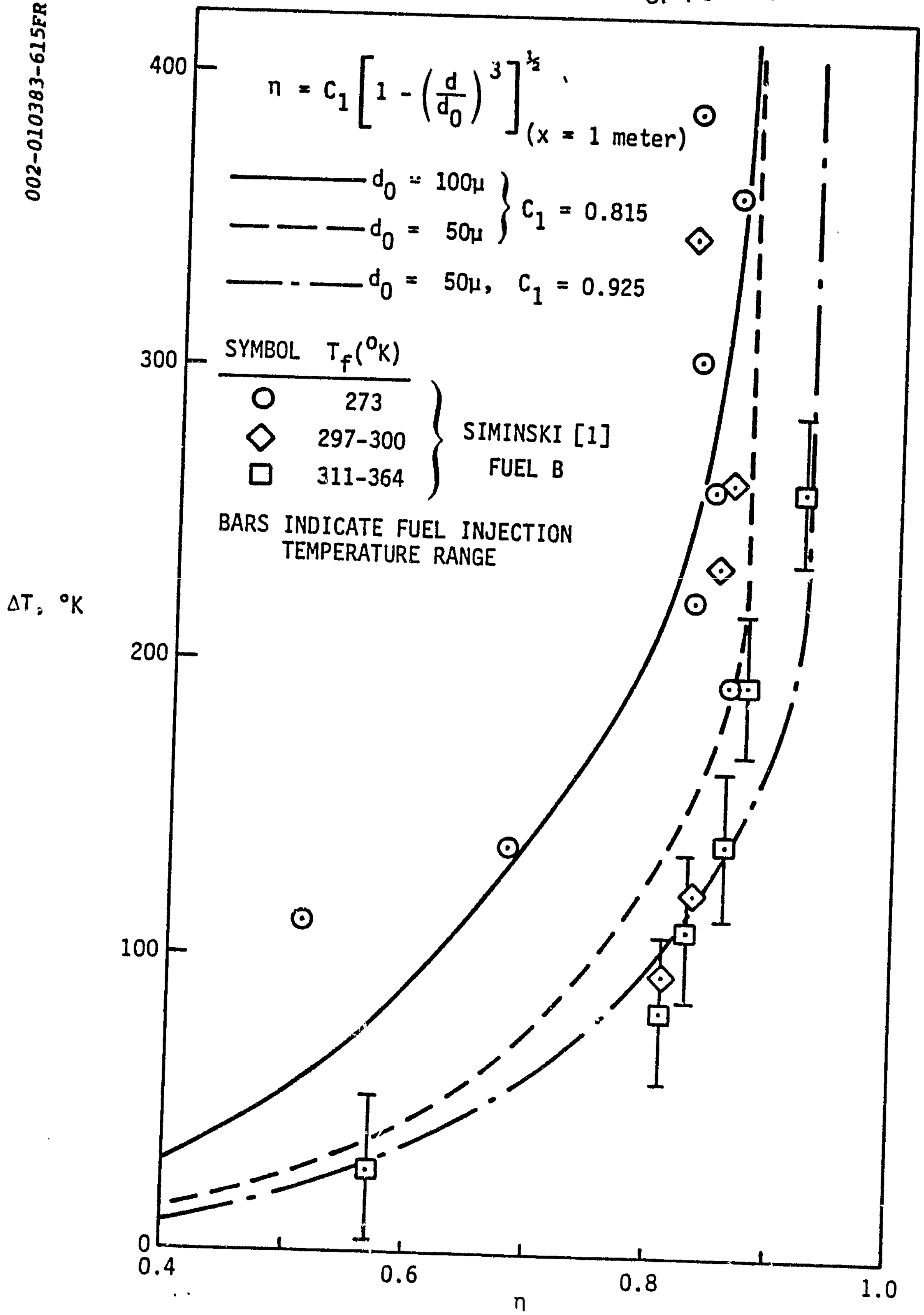

FIGURE 2. Correlation Between Vaporization Rate and Efficiency, Fuel B (Table 2).

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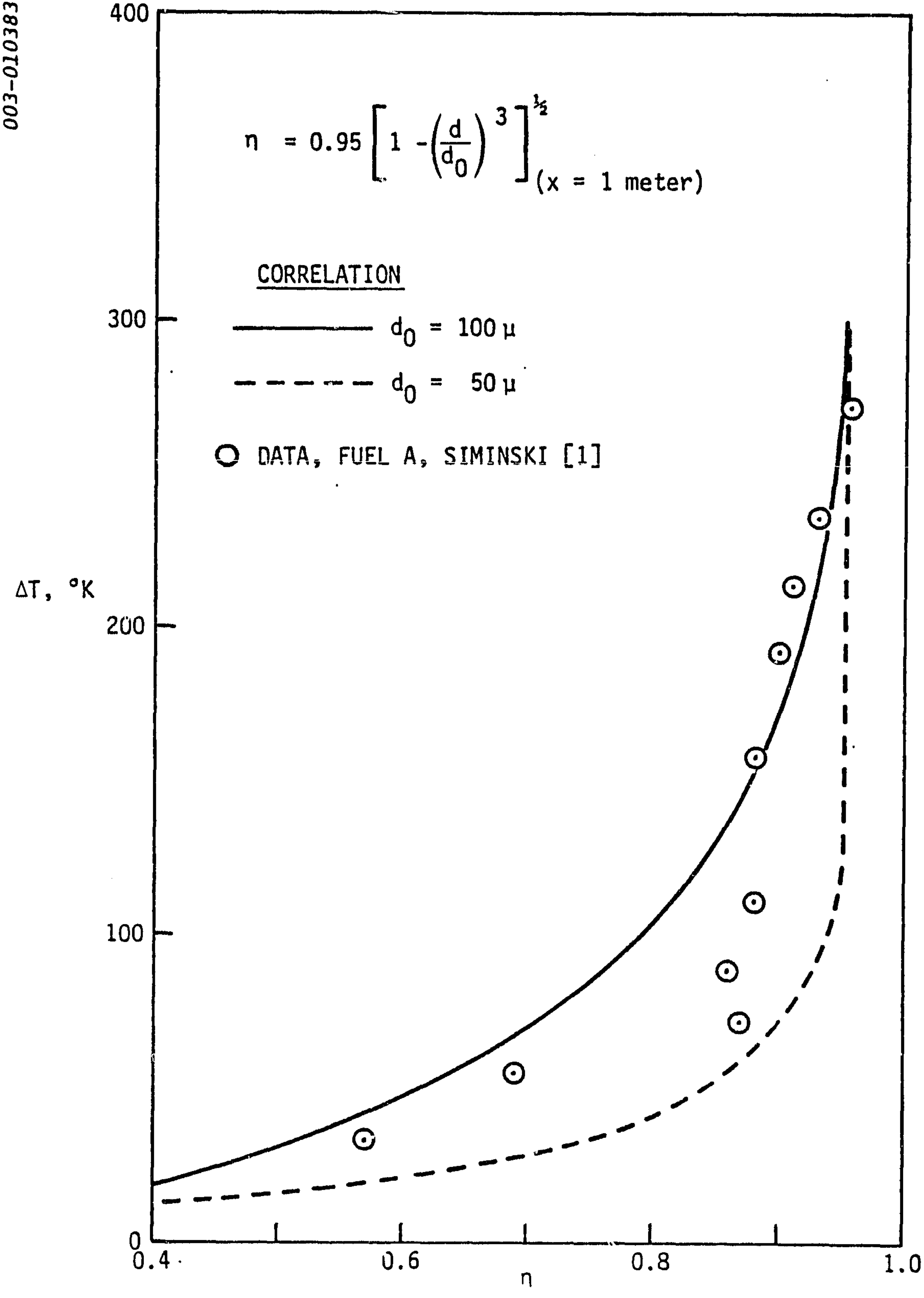

FIGURE 3. Correlation Between Vaporization Rate and Efficiency, Fuel A (Table 2).

has been directed toward the development of empirical correlations. While such empirical correlations are in general limited by the range of variables considered, and to a relatively small range of fuel properties, they do provide some insight into the effects of fuel property variations on each of these processes. For example, the volatility of the fuel, discussed in Section 2.1.2, is the key parameter that enters the correlation between η and the vaporization rate that yields the results shown on Figs. 2 and 3. This correlation thus provides direct evidence of a link between fuel property variation and overall burner performance.

2.1.1 Droplet and Spray Formation

Numerous investigations of the droplet and spray formation processes have been carried out, with applications ranging from industrial burners through gas turbine combustors, to rocket injectors. These investigations have resulted in the development of a variety of correlations for both droplet size and spray distribution for different injectors and types of fuels. For example, Ingebo and Foster [2] obtained an expression for volume - mean drop diameter $(d_{30})^*$ from experiments which involved five fluids (isooctane, water, carbon tetrachloride, kerosene, and benzene) and an air velocity range of 30 m/sec to 213 m/sec. The fuel was injected from a simple orifice injector mounted in a flat plate, and was injected at an angle of 90^0 to the airstream. These data led to the correlating expression

$$\frac{d_{30}}{d_0} = 3.9 \left(\frac{\sigma \mu_a}{\rho_a^2 V_a^3 {d_0}^2} \right)^{1/4} \qquad (6)$$

---

*In this discussion, the nomenclature d_{nm} will be used, where

$$d_{nm} = \left[\sum n_i d_i^n / \sum n_i d_i^m \right]^{1/(n-m)}$$

and n_i represents the number density (number/unit volume) of droplets having diameter d_i.

or

$$\frac{d_{30}}{d_0} = 3.9 \left(\frac{We}{Re}\right)^{1/4} \qquad (7)$$

where We is the Weber number based on drop diameter and Re the drop diameter Reynolds number. The terms σ, μ_a, ρ_a, and V_a appearing in Eq. 6 are the liquid surface tension, air dynamic viscosity, air density, and air velocity, respectively. In Eq's. (6) and (7) d_0 is the diameter of the injection orifice. Since the Reynolds number appearing in Eq's. (6) and (7) is based on air stream properties, the only fuel property which appears is the fuel surface tension, and Eq. (6) indicates $d_{30} \propto \sigma^{1/4}$.

A second correlating expression is that given by Weiss and Worsham (quoted by Weiss and Morgenthaler [3]) which was derived from data obtained in experiments in which molten wax was injected from a coaxial injector into an airstream held at the same temperature as the wax. This expression, for the surface/volume mean diameter d_{32}, can be written

$$d_{32} = 0.61 \left(\frac{\sigma}{\rho_a V_R^2}\right) \left(\frac{V_R \mu_L}{\sigma}\right)^{2/3} \left(1 + 10^3 \frac{\rho_a}{\rho_L}\right) \left(\dot{m}_L \frac{\rho_L \sigma \mu_a}{\mu_L^4}\right)^{1/12} \qquad (8)$$

in which $\dot{m}_L$ is the liquid flow rate, μ_L the liquid dynamic viscosity, and V_R the (absolute) relative velocity between liquid and air stream. The remaining symbols are as previously defined. Note that Eq. (8) indicates that $d_{32} \propto \sigma_L^{5/12}$, which is almost the square of the relationship implied by Eq. (6); moreover, this expression indicates a relatively strong dependence of d_{32} on fuel viscosity, $\mu_L : d_{32} \propto \mu_L^{1/3}$. Fuel viscosity does not appear in the correlation given by Eq. (6). Eq. (8) also shows a strong influence of gas-stream/droplet relative velocity, V_R, on $d_{32} : d_{32} \propto V_R^{-4/3}$. This provides an indication of the influence of aerodynamic effects that in general do not scale in the same manner as do the liquid phase phenomena. It is also of interest to note that σ, ρ_L, and μ_A were not varied in the experiments which led to Eq. (8), so that the variations in d_{32} with these properties embodied in Eq. (6) are basically conjectural.

A third correlation, applicable to injection from an air-assist-type atomizer, is that proposed by Nukiyama and Tanasawa [4].

$$d_{32} = 585\left(\frac{\sigma}{\rho_L V_R^2}\right)^{0.5} + 597\left(\frac{\mu_L{}^2}{\sigma\rho_L}\right)^{0.225}\left(\frac{10^{-3}\rho_L V_L}{\rho_a V_a}\right)^{1.5} \tag{9}$$

where V_L and V_a are the liquid airstream velocities, respectively, and V_R, as in Eq. (8), is the relative velocity between the liquid stream and air stream. Unlike Eq's. (6) and (8), Eq. (9) is not dimensionally homogeneous. The units to be used for the terms appearing in Eq. (9) are as given in Table 3. The resulting diameter is in microns.

TABLE 3

UNITS FOR NUKIYAMA & TANASAWA DROP SIZE EXPRESSION [4]

Term	Definition	Dimensions	Range Considered In Developing Correlation
ρ_L	Liquid Density	g/cm^3	0.7 - 1.2
μ_L	Liquid Viscosity	cp	0.3 - 50
σ	Surface Tension	dynes/cm	19 - 73
ρ_a	Air Density	g/cm^3	N/A
V_R	Relative Velocity	m/sec	N/A
V_L	Liquid Velocity	m/sec	N/A

The drop size expression given by Eq. (9) has the general form

$$d_{32} = \left(d_{32}\right)_1 + \left(d_{32}\right)_2$$

where $(d_{32})_1$ is dominated by relative velocity $[(d_{32})_1 \propto V_R^{-1}]$ and $(d_{32})_2$ is dominated by liquid viscosity: $(d_{32}) \propto \mu_L^{0.45}$. Both of these variations are not greatly different from those embodied in the expression given by Weiss and Worsham [Eq. (8)], but in Eq. (9) they appear as additive terms rather than as a product as in Eq. (8). Note further that the Nukiyama and Tanasawa expression [Eq. (9)] does not indicate any effect of nozzle diameter, d_0, on the resulting mean drop size.

A similar expression for surface/volume mean diameter (or Sauter mean diameter) was obtained by Lorenzetto and Lefebvre [5], but in this expression the nozzle diameter appears in the term for $(D_{32})_2$. The expression derived by Lorenzetto and Lefebvre is

$$d_{32} = 0.95 \left[\frac{(\sigma W_L)^{0.33}}{\rho_L^{0.37} \rho_a^{0.30} V_R} \right] \left(1 + \frac{W_L}{W_a}\right)^{1.70} + 0.13 \left(\frac{\mu_L^2 d_0}{\sigma \rho_L} \right)^{0.5} \left(1 + \frac{W_L}{W_a}\right)^{1.70} \qquad (10)$$

As was the case with respect to the expression developed by Nukiyama and Tanasawa, Eq. (10) is not dimensionless so that the value of the coefficient used in the expression depends on the units used for the various terms, and the resulting value of d_{32} is expressed in meters. The terms appearing in Eq. (10), their definition, and their dimensions are as given in Table 4.

TABLE 4

TERMS USED IN LORENZETTO AND LEFEBVRE EXPRESSIONS AND THEIR UNITS [5]

Term	Definition	Units
d_0	Fuel Orifice Diameter	Meters
V_R	Liquid-Gas Relative Velocity (absolute)	Meters/sec
W_a	Air Mass Flow Rate	kg/sec
W_L	Liquid Mass Flow Rate	kg/sec
μ_L	Liquid Dynamic Viscosity	kg/m-sec
ρ_a	Air Density	kg/m^3
ρ_L	Liquid Density	kg/m^3
σ_μ	Liquid Surface Tension	kg/sec^2

As was the case for the Nukiyama and Tanasawa correlation, the first part of Eq. (10) is dominated by the relative velocity: $(d_{32})_1 \propto V_R^{-1}$, while $(d_{32})_2$ is dominated by liquid viscosity: $(d_{32})_2 \propto \mu_L$. The dependence of $(d_{32})_2$ on μ_L is, however, considerably larger than that exhibited by the Nukiyama and Tanasawa expression, and Eq. (10) introduces a dependency of $(d_{32})_1$ on air density that is absent from Eq. (9).

Each of the correlations so far discussed has been developed for injection of fuel into an airstream, either from a plain orifice or using an air-assist atomizing nozzle. Correlations also exist for the droplet size produced by pressure atomizers in quiescent surroundings. One such correlation is that reported by Fraser [6]:

$$d_{32} = 220P^{-0.458}Q^{0.209}\nu_L^{0.215} \tag{11}$$

in which d_{32} is in microns, P, the nozzle pressure, is in lb/in^2, Q, the flow rate through the nozzle is in lb/hr, and ν_L, the kinematic viscosity, is in centistokes. Eq. (11) was derived from data obtained for a fairly large variety of fuels, most of which were fuels considered for gas turbine applications. Note that the only fuel property to appear in Eq. (11) is the kinematic viscosity, and the dependence of d_{32} on kinematic viscosity is relatively weak.

As is clear from the discussion to this point, there is a fair amount of variation in the importance given to various fuel properties in determining drop size in the existing drop size correlations. In an effort to provide some theoretical foundation for the definition of drop sizes resulting from liquid jet breakup, Adelberg [7] carried out a detailed analytical study of the breakup process. It is assumed in the formulation of the model that the relative velocity between fuel and airstreams is such that the process is one of ligament formation from the fuel jet and subsequent breakup of the fuel ligaments into droplets. Thus, the analysis concerns prediction of the characteristics of the surface waves on the liquid jet; part of the analysis involves determination of the minimum and maximum wavelengths which will grow on the jet surface. Since the ligament diameter is taken to be proportional to the wavelength of disturbance, and the drops are assumed to be equal in diameter to the ligament diameter, these minimum and maximum wavelengths are thus proportional to the minimum and maximum drop diameters produced by a given jet interaction process.

The frequency of ligament formation depends on the type of waves generated, and two types are considered by Adelberg [7]: capillary waves and acceleration waves. The former category involves a wave mechanism that is dominated by surface tension, while the latter is dominated by an acceleration force imposed by the interaction of the liquid jet and the freestream. As would be expected from the different mechanisms, different wavelengths are involved in the two processes so that the drop sizes produced also depend on the mechanism of formation. The resulting expression for the arithmetic mean drop diameter is

$$\overline{d}_\sigma \propto d_0^{1/2} \left[\frac{\mu_L (\sigma/\rho_L)^{1/2}}{\rho_a V_R^2} \right]^{1/3} \tag{12}$$

for the capillary wave region, while the expression for the arithmetic mean drop diameter for the acceleration wave region is

$$\overline{d}_a \quad \left[\frac{\mu_L (\sigma/\rho_L)^{1/2}}{\rho_a V_R^2} \right]^{2/3} \tag{13}$$

Note that the orifice diameter does not appear in the expression for the acceleration wave region. If the two terms that appear in the Nukiyama and Tanasawa, and Lorenzetto and Lefebvre correlations are identified with the capillary and acceleration wave regions on the basis of the appearance of the orifice diameter in the Lorenzetto and Lefebvre expression for $(d_{32})_2$, a comparison of the fuel property dependencies expressed by Eq's. (12) and (13) with those inherent in the empirical correlations so far discussed is as listed in Table 5.

TABLE 5

COMPARISON OF EMPIRICAL DROP DIAMETER DEPENDENCY ON FUEL PROPERTIES WITH THAT IMPLIED BY THEORETICAL ANALYSIS OF THE DROP FORMATION PROCESS

	Exponents							
	Experimental Correlation							
			Nukiyama and Tanasawa [4]		Lorenzetto and Lefebvre [5]		Theory (6,7)	
Variable	Ingebo and Foster [2]	Weiss and Worsham [3]	Capillary	Acceleration	Capillary	Acceleration	Capillary	Acceleration
Surface tension	1/4	5/12	1/2	-0.225	0.33	-1/2	1/6	1/3
Liquid viscosity	0	1/3	0	.450	0	1	1/3	2/3
Liquid density	0	−1/12	-1/2	1.275	-0.37	-1/2	-1/6	-1/3

Recognizing that a variety of different fuel injection schemes are represented by empirical correlations involved in Table 5, and that of these, that of Weiss and Worsham is closest to the configuration considered by Adelber in developing the theoretical formulation, it remains evident that theoretical considerations do not shed much light on the dependency of droplet size on fuel properties. There is clearly a need for a systematic study of the droplet formation process, even for conventional fuels. Such a systematic study is represented by the work described by Lefebvre [8], but this work is limited in scope to air-assist atomizers and gas turbine fuels. Recent work [9] has outlined computational approaches for the examination of the spray formation process at low Reynolds numbers; with the use of an appropriate Reynolds number scaling law this work could form the basis for techniques to be used to analyze the spray formation process and, in particular, fuel properties effects in more detail than has heretofore been possible.

Notwithstanding the parlous state of current drop size correlating expressions, it is possible to use the expressions outlined in this section to estimate the effects of fuel properties on fuel drop size. To carry out this estimation it is necessary to establish a baseline case which, for this work, has been defined using physical properties of No. 2 fuel oil as specified in Appendix A. Airflow and relative velocities have been specified arbitrarily, as have the air and fuel mass flows, the fuel injection pressure, and the nozzle orifice diameter, for those correlations which require values of these parameters. Note that the air flow represents only that through the nozzle itself. The values choses to form the baseline case are given in Table 6.

With the parameter values given in Table 6, the droplet diameter predictions listed in Table 7 result. While at first glance these results indicate substantial differences, if the pressure-atomizing nozzle result is ignored, the air-atomization results yield a mean droplet diameter of 208μ with a standard deviation of 71μ, despite the rather different applications for which most were devised. Thus, for comparison with the physical property sensitivities to be examined next, the spread in diameter values obtained using the different correlations discussed is from 0.66 to 1.34 of the mean droplet diameter.

The sensitivity to liquid density of the droplet diameter predictions produced by the four air-atomizing injection correlations described in this

TABLE 6

PARAMETERS FOR SENSITIVITY STUDY BASELINE CASE
(No. 2 Fuel Oil)

Parameter	Symbol	Units	Value
Liquid Viscosity	μ_L	kg/m-sec	2.15×10^{-3}
Liquid Density	ρ_L	kg/m^3	843.8
Surface Tension	σ	kg/sec^2	0.030
Air Viscosity	μ_a	kg/m-sec	1.66×10^{-4}
Air Density	ρ_a	kg/m^3	1.123
Air Velocity	V_a	m/sec	33.5
Relative Velocity	V_R	m/sec	30.5
Orifice Diameter	d_0	m	5×10^{-4}
Fuel Mass Flow	$\dot{m}_L, W_L$	kg/sec	6.47×10^{-3}
Air Mass Flow	W_a	kg/sec	2×10^{-2}
Fuel Injection Pressure	P	atm	10

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TABLE 7

BASELINE CASE (NO. 2 FUEL OIL) DROPLET DIAMETER PREDICTIONS

CORRELATION	APPLICATION	$d_{32}(\mu)$
Ingebo and Foster [2]	Normal injection from plain orifices into high speed air stream	287
Weiss and Worsham [3]	Coaxial injection from plain orifice into high speed air stream	184
Nukiyama and Tanasawa [4]	Injection from plain, air-assist atomizing nozzle	122
Lorenzetto and Lefebvre [5]	Injection from plain, air-assist atomizing nozzle.	240
Fraser [6]	Pressure-atomizer injection into quiescent surrounding	62

section is shown in Fig. 4. In addition to the four correlations already discussed, this figure includes the expression reported by Kurzius and Raab [10] for high speed flows

$$d_{32} = 61\mathrm{We}^{-3/8}(\mathrm{Re}/M_a)^{-1/4} \tag{14}$$

where

$$\mathrm{We} = \rho_L V_a^2 d_0/\sigma$$

$$\mathrm{Re} = \rho_a V_a d_0/\mu_a$$

and M_a is the airflow Mach number, $M_a \geq 1$. Except for the Ingebo and Foster expression (Ref. 2), which does not depend on liquid density, all of the expressions shown in Fig. 4 indicate a similar, and relatively strong liquid density dependence. However, as the data points also noted on Fig. 4 indicate, typical variations in liquid fuel density are small for fuels ranging from kerosene to SRC-II heavy distillate. Thus, these results indicate that the ultimate effect of fuel density variation on predicted drop size is well within the range of drop size predictions created by variations in available empirical drop size expressions. Only for fuels whose density is less than half that of No. 2 fuel oil does the effect of density become larger than the deviation inherent in available drop size correlations.

Surface tension is a parameter which enters all of the air-atomization droplet size correlations discussed in this section, so that the strong sensitivity of droplet-size expressions to this parameter, shown in Fig. 5, is not surprising. Here there is considerably more variation between correlations than was observed in Fig. 4, but almost all of the correlating expressions indicate that physically realizable values of liquid surface tension can result in drop size effects larger than the variation observed between correlations. On the other hand, values of surface tension for liquid fuels such as No. 6 fuel oil and the mid- and heavy-distillates of SRC-II all cluster around that of No. 2 fuel oil, so that the range of values of surface tension observed with these fuels is not large compared to the differences observed between correlations.

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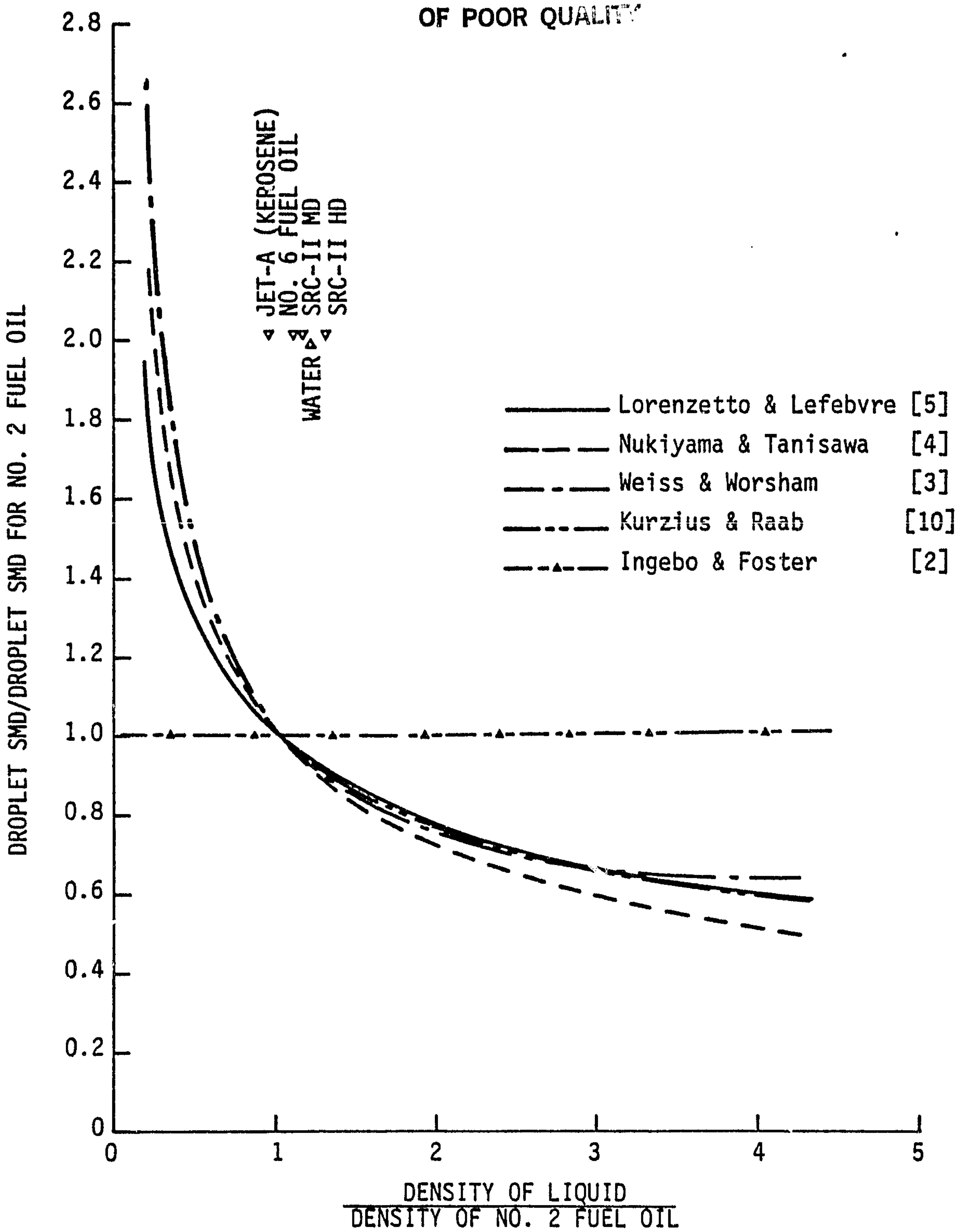

FIGURE 4. Sensitivity of Droplet Size to Liquid Density.

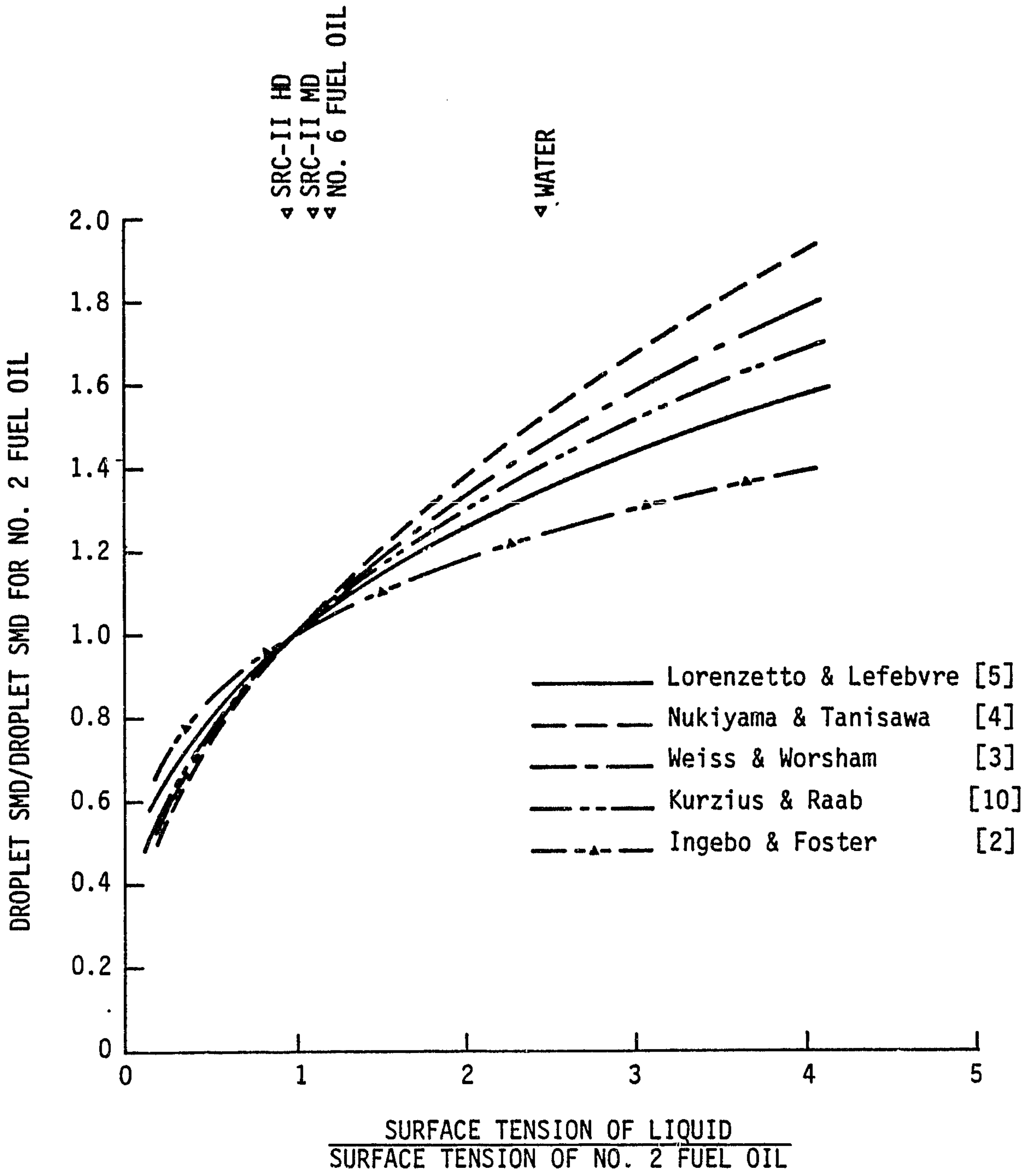

FIGURE 5. Sensitivity of Droplet Size Prediction to Surface Tension.

Liquid viscosity variations do not affect the drop size predicted by any of the correlations except the Weiss and Worsham correlation [3] and the Fraser correlation [6], as is shown by the results presented in Fig. 6. Liquid viscosity was not varied in the experiments that form the basis for the Weiss and Worsham expression; instead, the power dependency inherent in that correlation arises from the use of the liquid viscosity in forming nondimensional groups. On the other hand, liquid viscosity was varied in developing the correlation for pressure-atomizing nozzles described by Fraser, and this correlation indicates* a relatively strong effect of fluid viscosity. This variation, coupled with the large potential changes in liquid viscosity that may occur with alternative fuels (as, for example, the SRC-II heavy distillate noted in Fig 6) indicates that for the pressure atomization process viscosity is a significant parameter. However, the results shown by Fig. 6 also indicate that where air-assist atomization is concerned, the effects of liquid viscosity are considerably smaller.

The analysis outlined in this section shows that, based on currently available drop size correlations, liquid viscosity and surface tension are the most significant fuel physical properties involved in determining drop size. Substantial variations in drop size with density occur only for density values well outside a range anticipated for fuels. For pressure atomization, liquid viscosity is apparently the dominant fuel property parameter, while for atomization through aerodynamic mechanisms, the liquid surface tension variation is the most significant. However, the range of drop size variation from correlation to correlation is nearly as large as that which can be expected from different fuel physical properties: there is a clear need for a systematic investigation of the processes involved in droplet and spray formation even for conventional fuels. This systematic investigation should include both experimental and analytical investigations, as one of the problems existant with current correlation expressions is their more-or-less general lack of theoretical foundation. Thus, the exponents that appear on the various properties that enter the correlating expressions arise from curve-fitting considerations

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*The correlation involves the kinematic viscosity ν_L. In developing Fig. 6, it was assumed that ρ_L = constant while varying ν_L to obtain different values of $\mu_L = \rho_L \nu_L$.

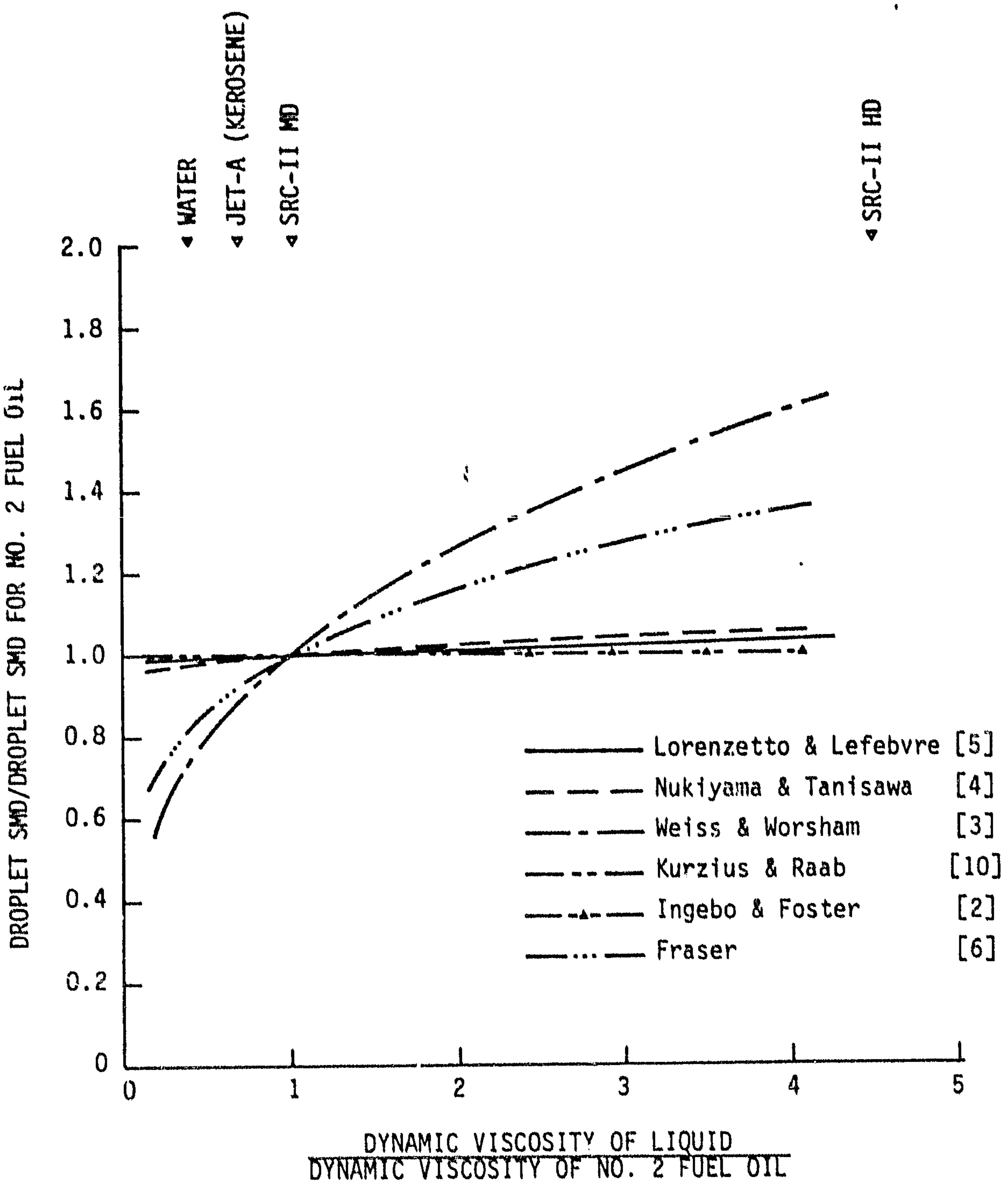

FIGURE 6. Sensitivity of Droplet Size Prediction
to Liquid Viscosity.

without theoretical underpinnings, making extrapolation of the results beyond the limits of physical property variation considered in developing each of the correlating expressions problematical.

2.1.2 Droplet Vaporization and Burning

The classical model of the comsumption of a spherical fuel drop burning in air involves the assumption that the rate-controlling process is molecular diffusion: chemical kinetic rates are assumed much faster than those associated with molecular diffusion phenomena. Effects of thermal diffusion and radiant heat transfer are neglected and the process is taken to be quasisteady. Then, if the fuel is considered to consist of a single component, and transport properties are assumed independent of temperature, a particularly simple closed-form solution is obtained:

$$\dot{m}_F = 4\pi r_L \frac{k}{C_p} \ell n(1 + B) \tag{15}$$

where k is the vapor thermal conductivity, C_p the average specific heat of the gas mixture and B is a transfer number given by

$$B \equiv \frac{1}{L}\left[\overline{C_p}\,(T_\infty - T_L) + \frac{QY_{0,\infty}}{i}\right] \tag{16}$$

in which T_∞ is the ambient temperature, T_L the droplet surface temperature, Q the fuel heat of combustion, L the latent heat of vaporization of the liquid per unit mass evaporating, $Y_{0,\infty}$ the ambient oxidizer mass fraction, and i the stoichiometric oxider/fuel mixture ratio. Then, since

$$\dot{m}_F = \frac{d}{dt}\left(\frac{4}{3}\pi r_L^3 \rho_L\right) \tag{17}$$

the solution given by Eq. (15) leads to the so-called "d^2" law (where $d=2r_L$), i.e.,

$$\frac{d[d^2]}{dt} = -\lambda \qquad (18)$$

where λ, the burning rate coefficient, is given by

$$\lambda = 8 \frac{k}{\rho_L \overline{C}_p} \ln (1 + B) \qquad (19)$$

Single drop experiments can be used to obtain values of the burning rate coefficient, λ, through measurements of the rate of change of droplet diameter with time. However, as can be seen from Eq. (19), λ is a strong function of temperature, as is also evident from the data shown in Fig. 7. These data, from Williams [11] all refer to droplets burning under natural convection conditions. Note that the higher molecular weight fuels appear to have a greater temperature dependence than neat hydrocarbons: Williams attributes this to enhanced radiant heat transfer because of liquid phase heat transfer. However, since the classical derivation that gives rise to the "d^2" law involves an assumption that the process is adiabatic, the enhanced heat transfer resulting from carbon formation also results in the "d^2" law failing as a descriptor of the process. In fact, for heavy hydrocarbon fuels the exponent n in a generalized "d^n" law is observed to be significantly less than 2. Nevertheless, despite these problems, empirical estimates of λ are useful for the assessment of the length of burner required to consume droplets of a given initial size, and can provide parametric comparisons that can be used to assess the effects of different fuel types on the combustion process in a given burner. A selection of available burning rate data is given in Table 8, from which it can be seen that there is a substantial variation in the empirical value of λ for different fuels. Since the time required to consume a droplet of initial size d_0 is, from Eq. (18)

$$t_b = d_0^2/\lambda \qquad (20)$$

it is clear from the data shown in Table 4 that consumption times and thus distances can vary by a factor of two.

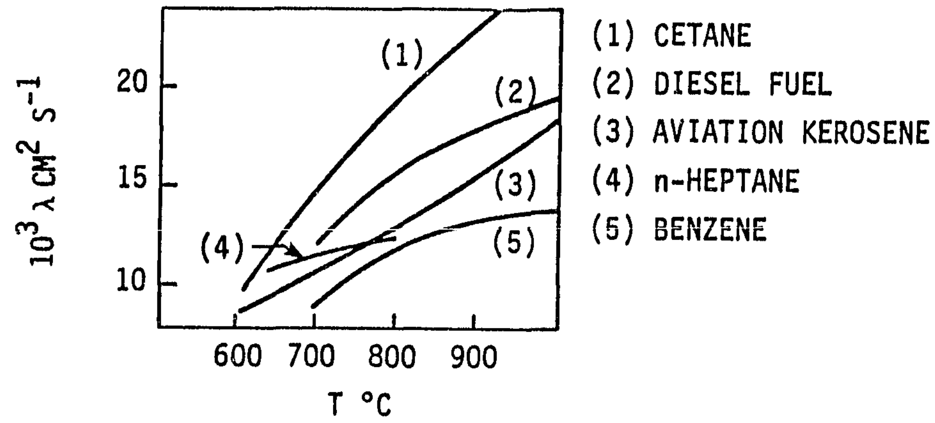

FIGURE 7. Burning Rate Coefficient of Compounds Burning in Air as a Function of Temperature. Data from Ref. 11.

Table 8. Burning Rate Coefficients for Fuels With Air at Room Temperature.

FUEL	λ $(10^{-3}\ cm^2\text{-}s^{-1})$	FUEL	λ $(10^{-3}\ cm^2\text{-}s^{-1})$
isopentane	11.2	butanol-1	7.2
2-pentane	11.2	propylene oxide	11.0
2:2 dimethyl butane	11.4	diethyl ether	10.8
iso-octane	9.5-10	acetone	10.6
benzene	9.5-9.9	furfuryl alcohol	7.2
toluene	6.6-7.7	amyl acetate	8.0
o-xylene	7.9	$2{:}2^1$-oxy diethanol	6.8,7.5
p-xylene	7.7	hydrazine	21.2,16.0
ethyl benzene	8.6	UDMH	11.0
isopropyl benzene	7.8	nitromethane	10.9
n-butyl benzene	8.6	acrilonitrile	10.2
t-butyl benzene	7.7	carbon disulfide	9.5
t-amyl benzene	7.8	butyl silane	14.1
pseudocumene	8.7	sulfur	5
cyclohexane	9.1	petroleum ether*	9.9
methyl cyclohexane	9.1	kerosene	9.2-10.2
tetralin	7.6	RP-1	7.8
methyl alcohol	8.6	diesel oil	7.9
ethyl alcohol	7.0-9.6	JP-4	8.7,10.4

*measured at 100-120°C

The estimate of droplet burning time made using Eq. (20), while useful for parametric comparisons and perhaps initial sizing, ignores the variations in velocity and temperature fields observed in a typical combustor and their effect on droplet lifetimes. To obtain a more refined estimate of droplet lifetime, the droplet trajectory equations must be solved for an ambient typical of that which is expected within the combustor. This solution, coupled to a point-by-point evaluation of λ from Eq. (19) will then provide a computation of both the droplet lifetime and the droplet trajectory. The droplet trajectory equations for an axisymmetric, swirling flowfield can be expressed by the set:

$$U_p \frac{dU_p}{dx} = \frac{3}{4} \frac{\mu}{\rho_p} \frac{C_d Re}{d^2} [U_g - U_p] \tag{21}$$

$$V_p \frac{dV_p}{dr} = \frac{3}{4} \frac{\mu}{\rho_p} \frac{C_d Re}{d^2} (V_g - V_p) + \frac{W_p^2}{r} \tag{22}$$

$$W_p \frac{dW_p}{d\theta} = \frac{3}{4} \frac{\mu}{\rho_p} \frac{C_d Re}{d^2} (W_g - W_p) - V_p W_p \tag{23}$$

In these expressions, U_p, V_p, and W_p are the axial, radial, and tangential (i.e., x, r, and θ) components of the droplet velocity; U_g, V_g, and W_g are similar components of the gas phase velocity; C_d is the droplet drag coefficient; μ the gas-phase viscosity; ρ_p the droplet density; Re is the local Reynolds number based on the droplet diameter and the slip velocity (i.e., $|U_g - U_p|$ in the case of the axial slip velocity Reynolds number) and d is the particle diameter. These expressions show that the rate of droplet equilibration with the gas flow for a given slip velocity can vary as $1/d^2$, indicating the sensitivity of the droplet trajectory to droplet size. The local droplet size is a function of the vaporization rate which is defined by consumption of droplet mass:

$$\frac{dm}{dt} = -\dot{m}_F \tag{24}$$

where $\dot{m}_F$ is the rate of consumption of the droplet, given, for example, by Eq. (15). The droplet temperature required to evaluate the vaporization rate is given by solution of the equation

$$mC_{p\ell}\frac{dT_L}{dt} = \pi d_p^2 h\,(T_g - T_L) - \dot{m}_F \sum_N j_i h_{\ell gi} + \dot{q}_r \tag{25}$$

where $C_{p\ell}$ is the liquid specific heat, h is the convective heat transfer coefficient, j_i is the i^{th} component of the volatized droplet mass, $h_{\ell gi}$ is the enthalpy of the volatized mass and $\dot{q}_r$ is the thermal energy absorbed by the droplet through radiation. To complete this system the change in the droplet composition is required and is expressible in terms of the liquid species conservation relations:

$$\frac{dM_i}{dt} = -j_i\dot{m}_F \tag{26}$$

For a droplet that can be treated as a single component (with a single boiling point temperature) it can be assumed (albeit as an extreme simplification of a complex process) that $\dot{m}_F = 0$ until $T_L = T_{BP}$; after the boiling point temperature is reached it can be assumed that all additional thermal energy added to the droplet provides the driving force for vaporization so $dT_L/dt = 0$ and $\dot{m}_F$ is given by Eq's. (15) and (16) with $T_L = T_{BP}$.

Two coefficients, the droplet drag coefficient C_d and the heat transfer coefficient h, are required to complete the model. In the absence of large mass transfer rates, the drag coefficient can be evaluated from available empirical data for inert spheres, yielding a relationship that, in general, involves only the relative Reynolds numbers, while the heat transfer coefficient involves the gas phase thermal conductivity and a Nusselt number correlation. The situation is more complicated when high mass transfer rates are encountered, since sufficiently high rates impact both the droplet drag and heat transfer rates. In the case of drag, for example, Eisenklam, et al. [12] have shown that the drag coefficient, C_D, is reduced in high mass transfer rate situations by the factor $(1 + B)$, where B is the transfer number given by Eq. (16).

From Eq's. (15)-(17), the fuel properties that impact droplet consumption processes are the vapor phase specific heat and thermal conductivity, the liquid density, and the fuel's heat of combustion and latent heat of vaporization. The burning rate coefficient is explicitly linearly dependent on the vapor-phase thermal conductivity and liquid density, and logarithmically related (through the transfer number B) to the heat of vaporization and heat of combustion. A somewhat more complicated relationship between vapor phase specific heat and burning rate coefficient exists, since both B and λ are functions of $\overline{C_p}$. Note also that mixture values of $\overline{C_p}$ and k are required for a fuel droplet burning in air. Oxygen is consumed in the flame sheet assumed to surround the droplet, but N_2 can diffuse to the droplet surface, so that the proper value of $\overline{C_p}$ and k required in the analysis is a function of both fuel vapor and N_2 concentration.

Evaluation of the sensitivity of burning rate coefficient to fuel property values is complicated by both the definition of $\overline{C_p}$ and its variation with temperature. If variations in $\overline{C_p}$ are assumed to be directly related to fuel property variation (i.e., $\overline{C_p} \propto C_{p\ fuel}$) and temperature variation is ignored, curves showing burning rate coefficient sensitivity to fuel property variation can be constructed. This has been carried out for three temperatures as shown on Fig. 8, with temperature variation of C_p ignored. (Thus, the different temperatures shown result in different values of (T_p-T_L) in the definition of B and, therefore, different impacts of a given fuel property variation). However,

C_p variation with T can be substantial as shown by the curve for nitrogen included as an inset in Fig. 8.

Even without consideration of the variation of C_p with temperature, the effects of C_p variation on burning rate are substantial, and the differences between the fuels shown are also substantial enough to indicate that a large variation in burning rate coefficient is to be expected. A similar situation exists for pure vaporization, which is described by Eq's. (15) and (16) with $Y_{0,\infty} = 0$. Thus, the results shown in Fig. 8 indicate that there is a need for data on vapor phase C_p (and thermal conductivity) of fuels as a function of temperature over a range of temperatures which correspond to those encountered in typical burner flowfields. Direct droplet burning rate measurements for alternative fuels are also required. However, as was the case for droplet size and spray formation phenomena, a need also exists for the updating of the experimental and analytical data base even for conventional fuels.

As was pointed out earlier in this section, the solution procedure that leads to the droplet consumption expressions given by Eq's. (15) and (16) is valid only for a very restricted set of circumstances. The droplet is assumed to consist of a single-component fuel at a single, uniform temperature; and a spherical flame sheet is assumed to exist around the droplet in which a one-step reaction between fuel and oxidizer to produce combustion products is assumed to take place. The process is assumed to be quasisteady. In practice, however, the fuel droplet is often multicomponent and a temperature gradient may exist within the drop, vapor-phase properties are functions of temperature, and finite-rate chemical reactions are taking place in a region surrounding the droplet. Finally, droplet vaporization and burning rates can be such that the quasisteady assumption does not apply. These effects all act to reduce the droplet consumption rate in general, and they are of particular importance for low volatility fuels in flowfields in which droplet heat-up time is significant relative to overall residence time. For liquids with high specific heats and low diffusivities, droplet internal transport processes are also important to the heat-up rate, as shown by Sirignano and Law, and by Sangiovanni in Ref. 13. Fig. 9 indicates the potentially large temperature variation that can occur in droplets of low thermal diffusivity liquid fuels.

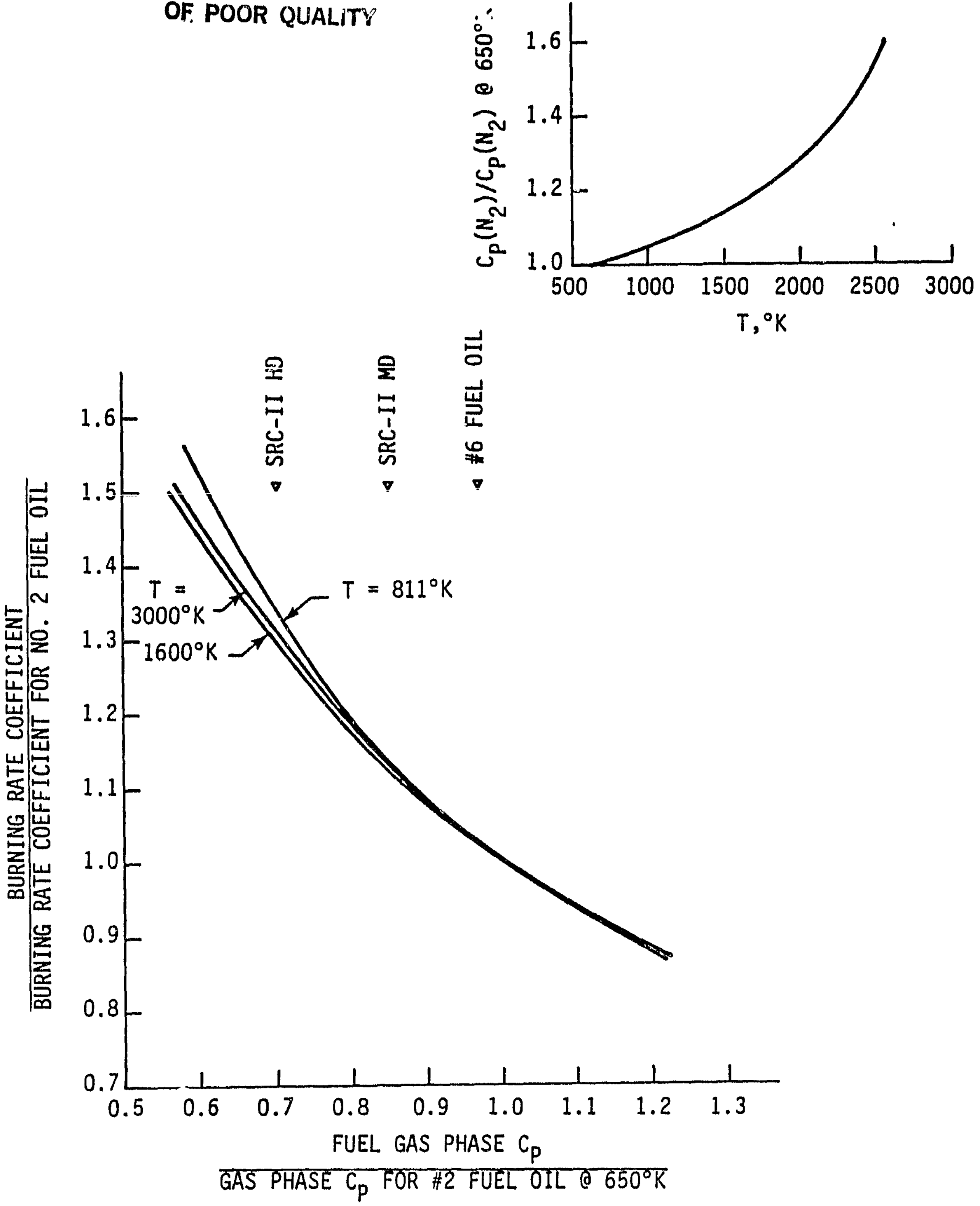

FIGURE 8. Variation in Burning Rate Coefficient With C_p Variation.

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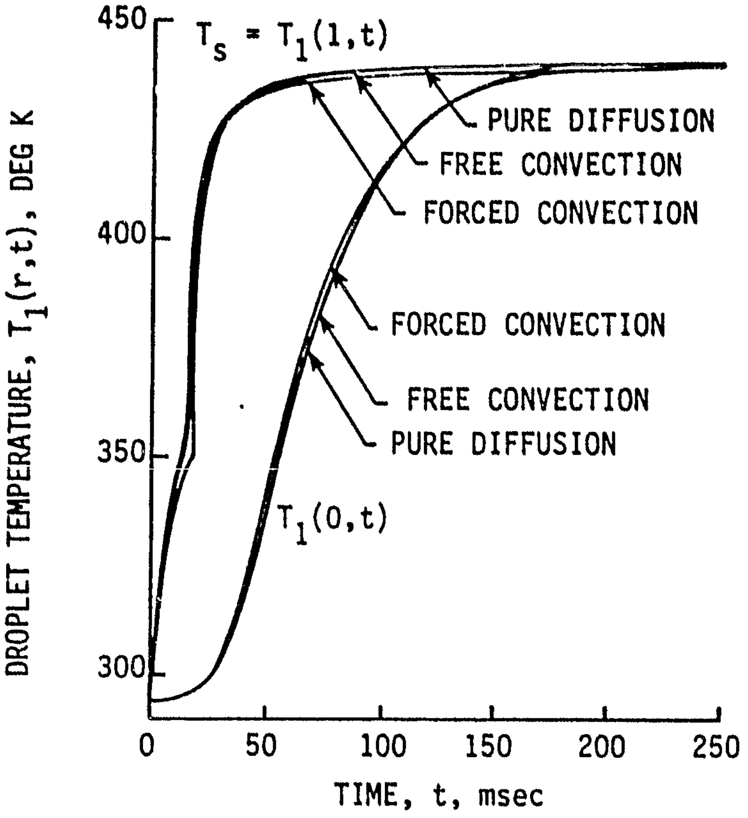

FIGURE 9. Variation of Droplet Center $[T_1(0,t)]$ and Surface $[T_1(1,t)]$ Temperatures With Time as a Function of Gas-Phase Transfer Mode. (Ignition and combustion of a 300-μ furfuryl alcohol droplet in air at 1400°K and 0.1355 g O_2/g air.)

Because of the restrictive assumptions used in deriving Eq's. (15)-(19), substitution of temperature-varying physical properties into these expressions is not strictly correct. Further, incorporation in the model of the effects of multicomponent fuels and finite rate chemistry can alter the solution considerably. In general, the incorporation of the effects of multicomponent fuels, finite rate chemistry, and variable properties leads to the need for a numerical solution procedure. However, little work has been done in this area or in the area of detailed modeling of the droplet and spray combustion process in general. The work that is required, both from the standpoint of alternate fuels design data bases and the utilization of more conventional fuels involves both experimental and analytical research into the mechanisms and phenomena involved in droplet combustion. Measurements of vapor phase specific heat and thermal conductivity, and of droplet burning rate coefficients, all as a function of temperature, are needed for both conventional and alternative fuels. These data would then provide a base for the development and verification of more complete models of droplet consumption phenomena, leading to the development of the techniques required to adequately examine the effects of alternative fuels on spray combustion.

2.2 Gas-Phase Fuel Combustion Characteristics

Gas-phase combustion characteristics include the processes of ignition and flame stabilization, the completion of combustion, and the production of soot and gas-phase emissions. Flame temperature and laminar flame speed are both quantities that are directly measurable and are directly related to the combustion process characteristics. The laminar flame speed itself is not of particular importance in industrial burner applications. The vast majority of industrial burner flowfields are turbulent, so that the actual flame speed is at least an order of magnitude higher than the laminar flame speed and dependent on the geometric and flowfield characteristics of the burner as well. However, laminar flame speed is a useful measure of the reactivity of a fuel, and laboratory experiments in which it is measured can provide some of the data necessary to determine fuel reaction rates.

Ignition and flame stabilization phenomena have been extensively studied in both gas-phase and multiphase flows. These phenomena, as well as those involved in combustion completion and emissions production, involve a closely coupled interaction between aerodynamic effects and the chemical kinetics of the reaction process. The physical properties of the fuel play an important role in the combustion processes considered in this section, since the heat of combustion of the fuel influences the flame temperature, effective reaction rates influence the ignition delay time and the residence time required for completion of combustion, and the fuel composition plays an important role in the characteristics of the species produced by combustion of the fuel and, thus, its emissions characteristics. On the other hand, fuel transport properties such as thermal conductivity and diffusivity are of only secondary importance in industrial applications because industrial burner flowfields are, in general, turbulent.

2.2.1 Ignition and Flame Stabilization

Continuous ignition of a flowing fuel-air mixture requires that the temperature of the unburnt fuel and air be raised to a sufficiently high value or that the mixture be in intimate contact with highly reactive intermediate species generated by a reaction zone in the vicinity of the incoming fresh mixture. Ignition delay time of a typical fuel is a strong function of temperature and fuel-air ratio, and can be of the order of milliseconds. Since residence times based on average flow-through velocities in an industrial burner can also be on the order of milliseconds, it is clear that some means of maintaining a high-temperature region within the burner in which residence times are sufficient for ignition and combustion initiation to take place is highly desirable. In most practical systems, this goal is achieved by back-feeding the products of combustion through the creation of recirculation zones.

Conceptually, there is little qualitative disagreement about the processes that are relevant to flame stabilization. Fig. 10 shows a schematic of a "bluff body" that typifies the classical method used to generate a recirculation zone. Once combustion is established in the near wake, hot products containing reactive intermediates are brought into contact with the fresh fuel-air mixture by the large scale recirculating eddies. The shear layer bounding the recirculation zone is a region of steep gradients in velocity, temperature, and concentration. Within this region the fresh fuel-air mixture is

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particle diameter. These expressions show that the rate of droplet equilibration with the gas flow for a given slip velocity can vary as $1/d^2$, indicating the sensitivity of the droplet trajectory to droplet size. The local droplet size is a function of the vaporization rate which is defined by consumption of droplet mass:

$$\frac{dm}{dt} = -\dot{m}_F \tag{24}$$

where $\dot{m}_F$ is the rate of consumption of the droplet, given, for example, by Eq. (15). The droplet temperature required to evaluate the vaporization rate is given by solution of the equation

$$mC_{p\ell} \frac{dT_L}{dt} = \pi d_p^2 h \, (T_g - T_L) - \dot{m}_F \sum_N j_i h_{\ell gi} + \dot{q}_r \tag{25}$$

where $C_{p\ell}$ is the liquid specific heat, h is the convective heat transfer coefficient, j_i is the i^{th} component of the volatized droplet mass, $h_{\ell gi}$ is the enthalpy of the volatized mass and $\dot{q}_r$ is the thermal energy absorbed by the droplet through radiation. To complete this system the change in the droplet composition is required and is expressible in terms of the liquid species conservation relations:

$$\frac{dM_i}{dt} = -j_i \dot{m}_F \tag{26}$$

For a droplet that can be treated as a single component (with a single boiling point temperature) it can be assumed (albeit as an extreme simplification of a complex process) that $\dot{m}_F = 0$ until $T_L = T_{BP}$; after the boiling point temperature is reached it can be assumed that all additional thermal energy added to the droplet provides the driving force for vaporization so $dT_L/dt = 0$ and $\dot{m}_F$ is given by Eq's. (15) and (16) with $T_L = T_{BP}$.

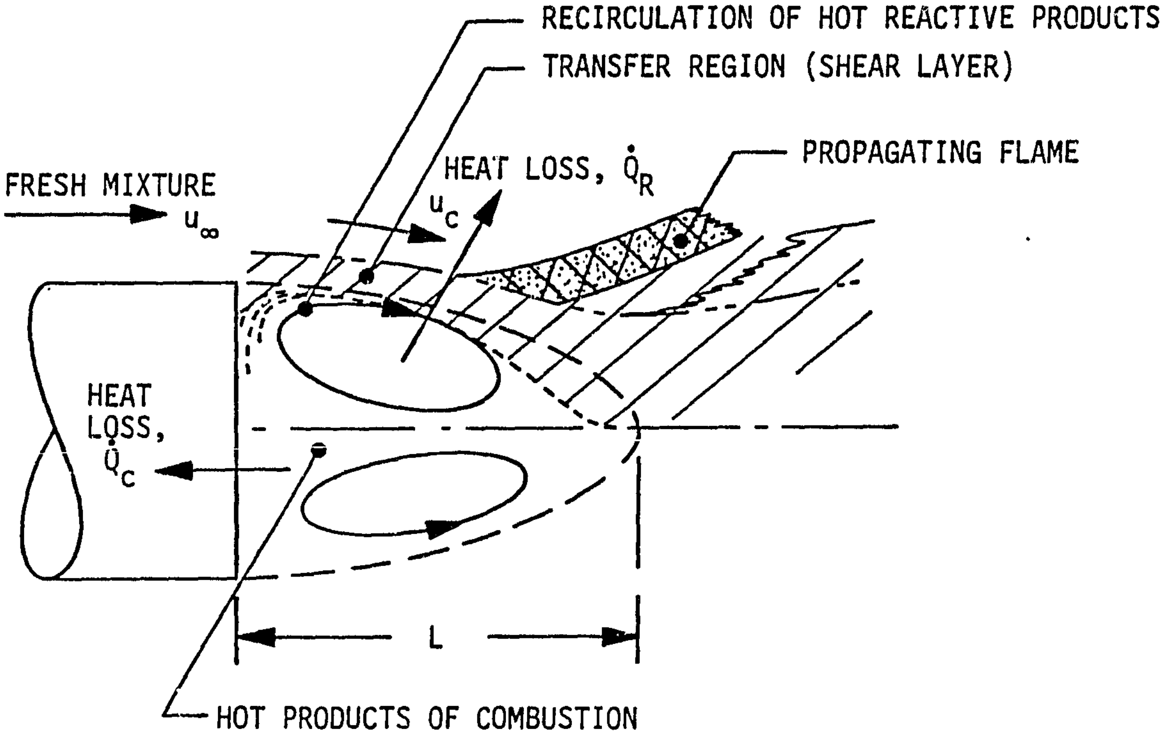


FIGURE 10. Schematic of Bluff Body Flame Stabilizer.

ignited. The transport of heat and mass into and out of the recirculation zone occurs in this transfer region, and the rate of transport determines the effectiveness of the flameholder in igniting the fresh mixture. Marble and Zukowski [14] described this process in simple terms by noting that ignition will occur if the contact time (i.e., the ratio of the recirculation zone length, L, to the contact velocity, U_c) is greater than the ignition delay time, τ_{ID}, of the fresh mixture. This relationship introduces reactivity properties of the fuel-air mixture and a geometric characteristic of the flameholder. The flame stabilization criterion given by Marble and Zukowski is simply:

$$\left.\begin{array}{l} \dfrac{U_c \tau_{ID}}{L} < 1, \text{ flame stable} \\ \\ \dfrac{U_c \tau_{ID}}{L} \geq 1, \text{ flame blows out} \end{array}\right\} \qquad (27)$$

The Marble and Zukowski criterion is a characteristic time formulation and is simple to use, provided that the contact time and ignition delay times can be evaluated. However, while it is intended to provide an indication of whether or not a flame will propagate into the fresh mixture, it does not directly reflect the performance of the combustion process in the body of the recirculation zone. Furthermore, it also involves an implicit assumption that the combustion process is confined to the transfer region surrounding the recirculation zone (Fig. 10). Nevertheless, the concept of characteristic times is an important one with respect to the correlation of flame stability data, and it has been exploited in a considerable body of recent work by Mellor and coworkers. For example, Plee and Mellor [15] have investigated a variety of axisymmetric flameholder configurations and have been successful in correlating stability using characteristic time parameters representing a "shear layer mixing time"

$$\tau_{s\ell} \propto D_f/U_\ell \qquad (28)$$

where D_f is a characteristic flameholder dimension and U_ℓ is the velocity at the lip of the flameholder, and a "chemical time"

$$\tau_{hc} = \frac{10^{-4}}{\phi} \frac{T_{s\ell}}{T} \exp\left(-21000/RT_{s\ell}\right) \qquad (29)$$

where $T_{s\ell}$ is a characteristic (hot) shear layer temperature, and ϕ and T are the equivalence ratio and temperature in the oncoming (premixed) stream. R is the universal gas constant. An example of this correlation, for propane-air mixtures, is shown in Fig. 11.

A second approach to the characterization of flame stability, based on the work of Longwell [16] and DeZubay [17], focuses attention on the recirculation zone volume. The experimental results obtained by Longwell and by DeZubay could be correlated by a dimensional parameter, Φ_{BO}, that is directly related to velocity and inversely to the product of the pressure and a characteristic dimension of the flameholder:

$$\Phi_{BO} \propto \frac{U_o^{\alpha}}{P_o^{\beta} D^{\gamma}} \qquad (30)$$

where U_o is the approach velocity, P_o the static pressure and D a characteristic flameholder dimension. The exponents α, β, and γ are expected to constant; Φ_{BO} as written is intended to serve as a correlating parameter for a given stream temperature and fuel type.

The concept embodied in Eq. (30) was extended by Ozawa [18], who reviewed a large amount of experimental data and found that the equivalence ratio at blowout for all these data could be related to a parameter of the form of Eq. (30) if the effect of temperature was also introduced. This correlation is shown in Fig. 12, from which the substantial effect of temperature can be seen. Note that a fairly wide variety of flameholder geometries were considered, which led to the introduction of an "effective diameter" in order to obtain the correlation, but the fuel used was in all cases kerosene; the results are shown in Fig. 12 compared to similar results obtained using a disc geometry and propane fuel.

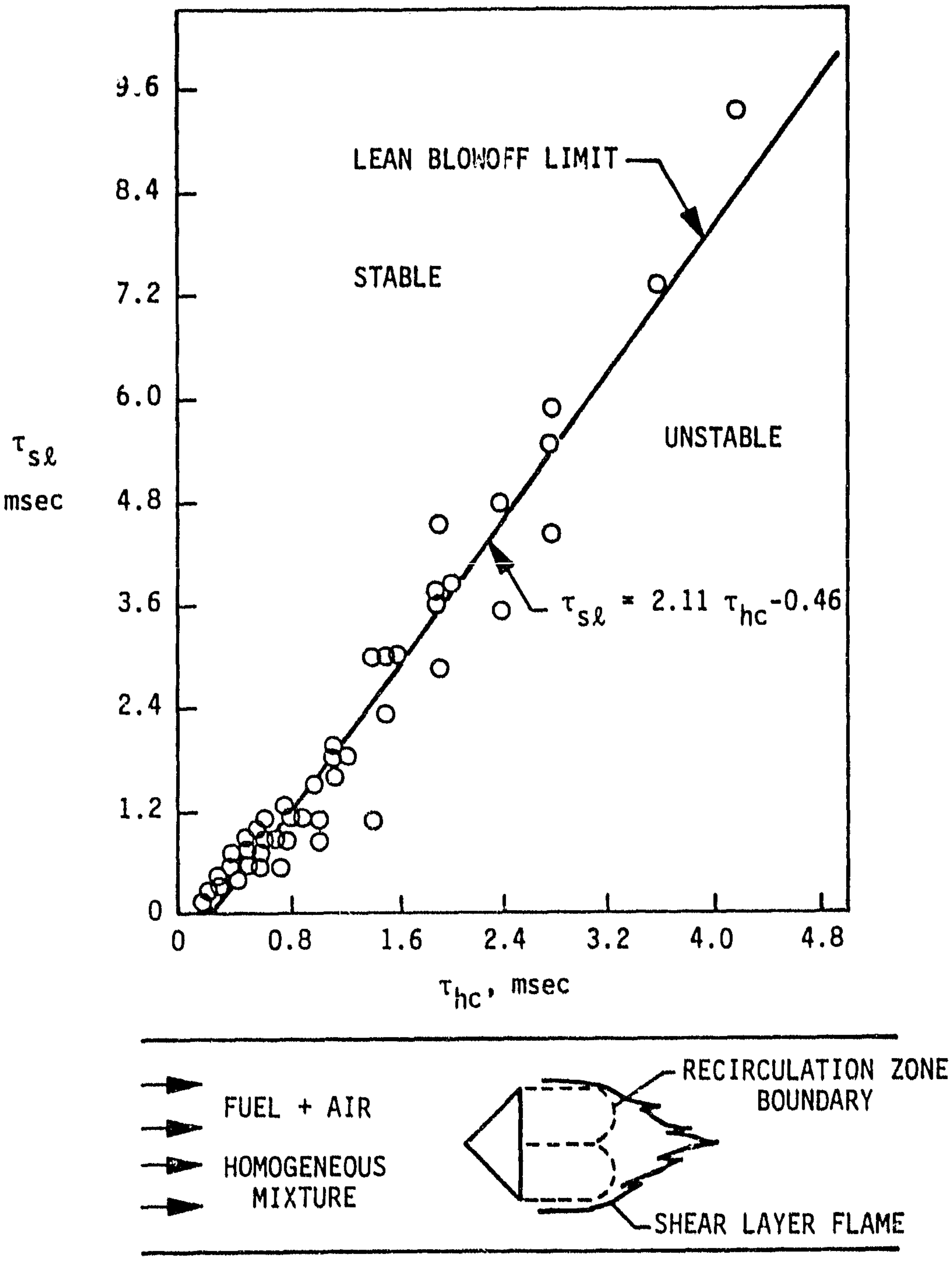


FIGURE 11. Characteristic Time Correlation for Baffle Flameholder; Propane Fuel.

SYM	FLAMEHOLDER	$\frac{d_e}{d}$	FUEL	MIXTURE TEMP (°R)	PRESSURE (atm)	NOTES
—	DISKS	1.6	PROPANE	550	1/3 TO 1	MEAN CURVE
◆	DISKS	1.6	KEROSENE	1030	~1	WIDE DATA SCATTER
▲	90° CONES	1.4	KEROSENE	1030	~1	
■	HEMISPHERES	1.1	KEROSENE	1030	~1	
●	60° V-GUTTER	1.73	KEROSENE	900	~1	APPROACH ε ~ 2.5%
◇	60° V-GUTTER	1.73	KEROSENE	900	~1	APPROACH ε ~ 10%
△	90° V-GUTTER	1.86	KEROSENE	1390	~1	
□	½ ROUND CHANNEL	1.46	KEROSENE	1390	~1	
○	CYLINDER	1.33	KEROSENE	1390	~1	TRANSVERSE FLOW

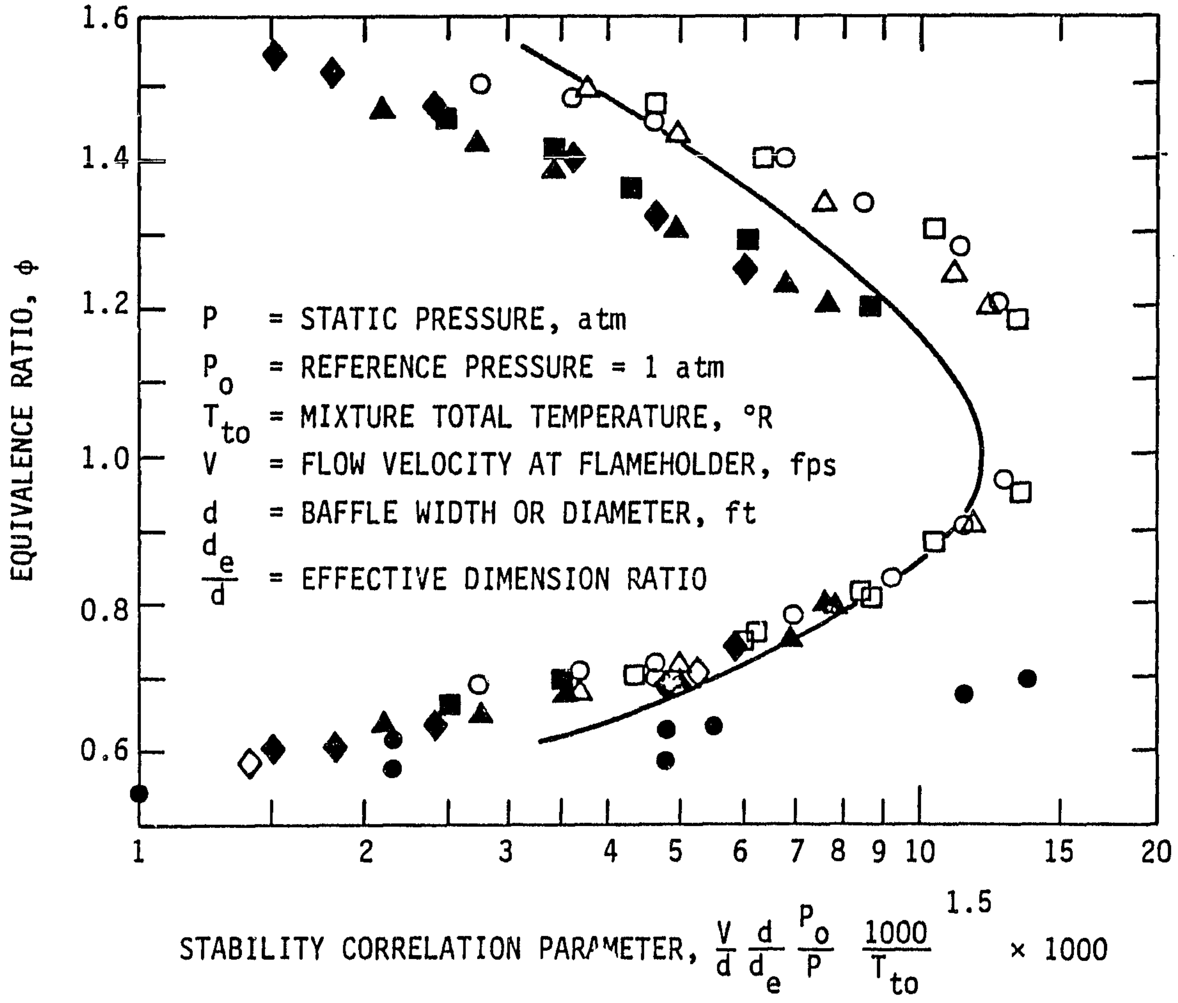


FIGURE 12. Baffle Stability Correlation
(From Ozawa [18]).

With the exception of the strong effect of chemical kinetics implied by the strong temperature dependency observed, effects of fuel properties are not explicit in either the characteristic time formulation or the blowout formulation based on Eq. (30), partly because the examples discussed have been concerned primarily with premixed, prevaporized systems. Fuel effects could be expected to be more important in nonpremixed and heterogeneous systems since (for turbulent flows, at least) the primary impact of fuel properties is on the spray formation, vaporization, and droplet burning processes. This expectation is borne out by the work reported by Ballal and Lefebvre [19], in which data for the range of fuels given in Table 9 was obtained. Several different hollow-cone flame stabilizers, with centrally-mounted spray injectors, were used in the work described in Ref. 19, and measurements were carried out at four different levels of oncoming-stream turbulence intensity.

TABLE 9

FUELS USED BY BALLAL AND LEFEBVRE [19]

Fuel	Stoichiometric Fuel/Air Ratio by Weight	Carbon/ Hydrogen Ratio	Specific Gravity at 293K	Kinematic Viscosity $m^2/sec \times 10^{-6}$	Spalding Transfer Number B
Isooctane	0.066	5.33	0.692	0.77	6.10
Kerosene	0.068	6.10	0.775	1.30	3.75
Gas Oil	0.068	6.40	0.837	5.00	3.10
Diesel Oil	0.070	7.00	0.900	14.50	2.80
Light Fuel Oil	0.072	7.40	0.930	165.00	2.50
Heavy Fuel Oil	0.073	7.70	0.970	860.00	1.50

Although a wide range of liquid viscosity is shown in Table 9, Ballal and Lefebvre used ten different simplex pressure atomizers to provide a controlled mean droplet size for the range of fuels considered, thereby precluding a direct evaluation of the effect of viscosity on flame stabilization. Surface tension effects are precluded for the same reason. However, the effect of volatility was included in the test series, as shown by the range of transfer numbers, which can be interpreted as characterizing the fuel volatility.

Ballal and Lefebvre [19] correlated their results for lean blowoff or weak extinction equivalence ratio, ϕ_{WE}, using stirred reactor theory, assuming that for the heterogeneous case the combustion process depends on the vapor phase fraction of the total fuel injected into the recirculation region, i.e.,

$$\phi_{WE}\text{ (heterogeneous)} = \phi_{WE}\text{ (premixed)}\cdot f^{-1} \tag{31}$$

where ϕ_{WE} (premixed) is as given by the expression

$$\phi_{WE}\text{ (premixed)} = C\left[\frac{\dot{m}_a}{VP^{1.25}\exp(T_o/150)}\right]^{0.16} \tag{32}$$

where $\dot{m}_a$ represents the air mass flow rate, V is the reaction volume, P the local pressure, and T_o is the inlet static temperature in ^oK. The vaporized fraction of the total fuel, f, is given by single droplet theory as discussed in Section 2.1.2, modified to account for convective augmentation of the droplet consumption rate. Thus,

$$f = 8.0\left(\frac{C_1}{C_3^3}\right)\left(\frac{\rho_a}{\rho_f}\right)\left(\frac{k}{C_p}\right)_a \ln\,(1+B)\left(\frac{V}{\dot{m}_a d_{32}^2}\right)\left(1 + 0.25C_2^{0.5}Re_{d_{32}}^{0.5}\right) \tag{33}$$

in which the subscript a refers to airstream quantities, and ρ_f is the density of the mixture within the flame stabilization zone. Two limiting forms of f can be defined. For $Re_{d_{32}} << 1.0$, which corresponds to a low pressure, low turbulence liquid,

$$f = 8.0 \left(\frac{C_1}{C_3^3}\right) \left(\frac{\rho_a}{\rho_f}\right) \left(\frac{k}{C_p}\right)_a \ell n\ (1+B) \left(\frac{V}{\dot{m}_a d_{32}^2}\right) \qquad (34)$$

while for $Re_{d_{32}} >> 1$ (high pressure, high turbulence)

$$f = \frac{2.0}{P} \left(\frac{C_1 C_2^{0.5}}{C_3^3}\right) \left(\frac{\rho_a}{\rho_f}\right) \ell n\ (1+B) V \left[\left(\frac{T_u}{100}\right) \frac{\mu_a}{\dot{m}_a d_{32}^2 A}\right]^{1/2} \qquad (35)$$

In devising Eq. (35), the Reynolds number has been assumed to be based on a relative velocity given by the turbulent rms velocity* and the rms velocity is given by

$$rms = u' = \frac{T_u}{100} U \qquad (36)$$

In Eq. (35), A is the area of the duct in which the flame stabilizer is located. In these expressions the surface-volume (or Sauter) mean diameter is used to characterize the actual polydisperse spray. However, different diameters characterize processes such as mass and momentum transfer, and this has been accounted for by the incorporation of the coefficients C_1, C_2, and C_3. Values of these coefficients for atomizers of the simplex and airblast type are 0.31, 0.21, and 0.46, respectively. (For monodisperse sprays, $C_1 = C_2 = C_3 = 1.0$, by definition).

In highly turbulent well-stirred regions the weak extinction equivalence ratio is given by

---

*thus, it is assumed that droplets follow the mean flow but not the turbulent fluctuation.

$$\phi_{WE} = C \left[\frac{\dot{m}_a}{VP^{1.25} \exp \frac{T_o}{150}}\right]^{0.16} \left[\frac{\rho_f}{\rho_a V \ln(1+B)}\right] \left[\frac{\dot{m}_a d_{32}^2 A}{\frac{T_u}{100} \quad \mu_a}\right]^{0.5} \tag{37}$$

However, for baffle-stabilized flames the role of turbulence is more complex because it affects not only the rate of fuel evaporation, but also the rate of entrainment of air into the wake region. Either effect could predominate but, in general, ϕ_{WE} increases with turbulent intensity for fuels of low volatility. Ballal and Lefebvre [19] developed the entrainment ratio expression given by

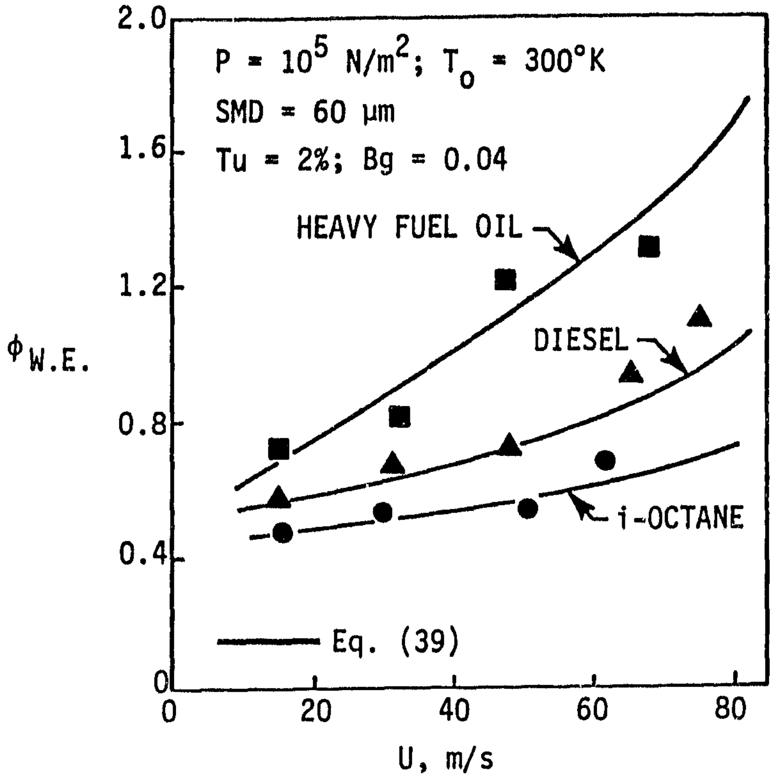
$$E = \frac{\dot{m}_a(\text{entrained})}{\dot{m}_a(\text{approach})} = C \left(\frac{B_g}{1-B_g}\right) (1+0.12\ T_u) \tag{38}$$

Identifying $\dot{m}_a$ in Eq. (37) as $\dot{m}_a$ (entrained), and replacing the reaction volume V with the expression $V = AB_g d$ relating the reaction volume to the overall duct area, A, blockage B_g, and flameholder characteristic dimension d yields, for baffle-stabilized flames

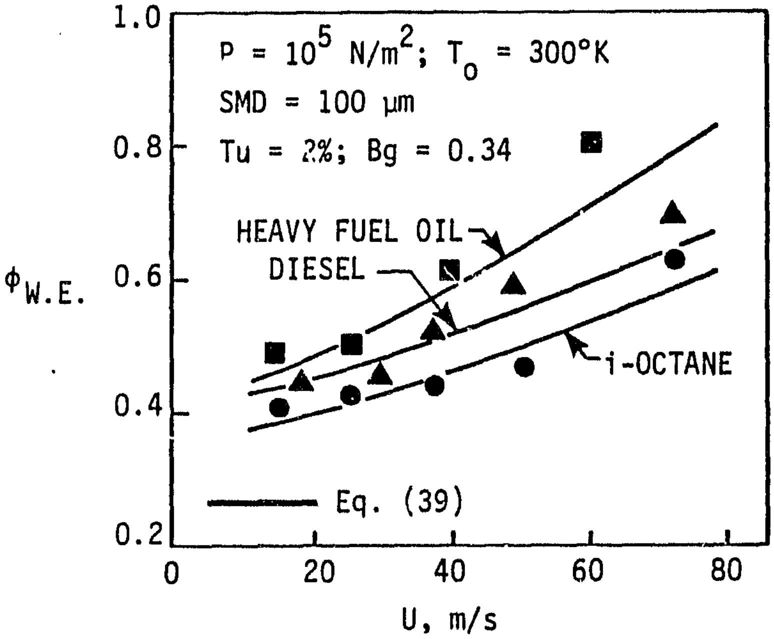
$$\phi_{WE} = \overline{C} \left[\frac{\rho_f}{d \ell n(1+B)}\right] \left[\frac{V d_{32}^3 (1+0.12 T_u)}{\rho_a \mu_a \frac{T_u}{100} \quad B_g(1-B_g)}\right]^{0.5} \left[\frac{V(1+0.12 T_u)}{P^{0.25} d(1-B_g) T_o \exp(T_o/150)}\right]^{0.16} \tag{39}$$

Fuel properties enter Eq. (39) through the transfer number B, the recirculation region characteristic density, ρ_f, and indirectly through d_{32}. Note that Eq. (39) indicates that $\phi_{WE} \propto \rho_f$: this direct dependency does not, however, imply a direct dependency on fuel properties since ρ_f is a result of the mixing and combustion process in the recirculation region.

The data used to develop Eq. (39) are shown in Figs. 13-18; a fit of Eq. (39) to all the data was accomplished with a value of C of 0.005. A general observation relative to the effects of fuel properties on flame stabilization is the relatively high level of sensitivity of ϕ_{WE} to fuel volatility. Most significant are the benefits realized with heavy, low volatility fuels through

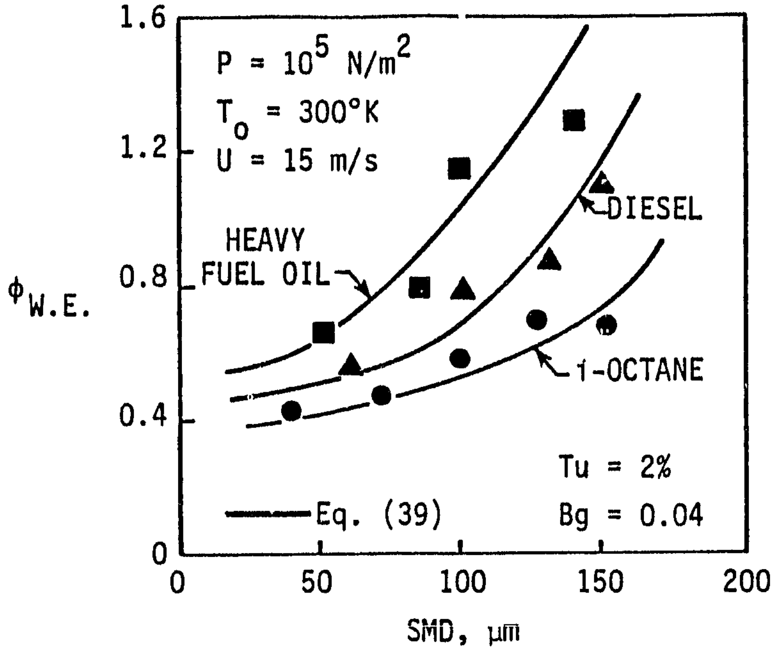


(a) Conical Baffle of Low Blockage Ratio

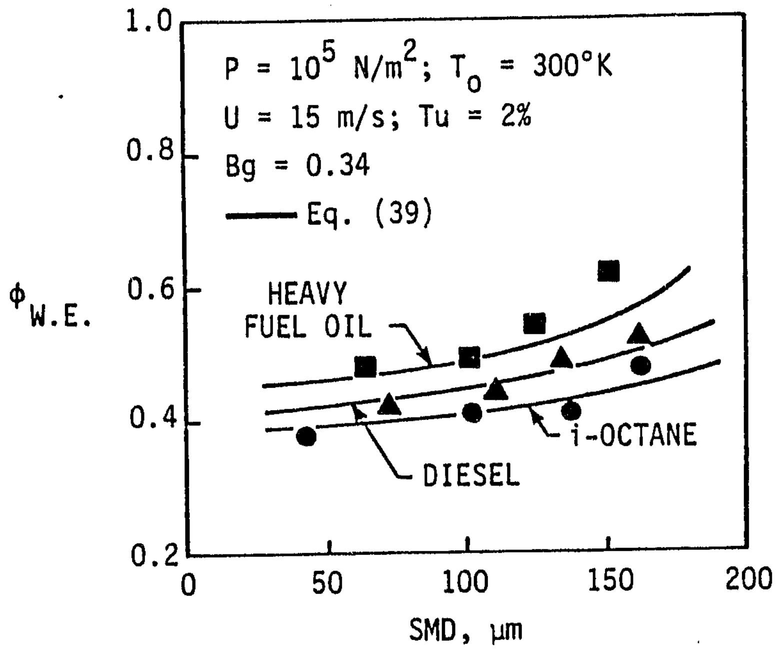


(b) High Blockage Ratio

FIGURE 13. Influence of Mainstream Velocity on Weak Extinction Limits.

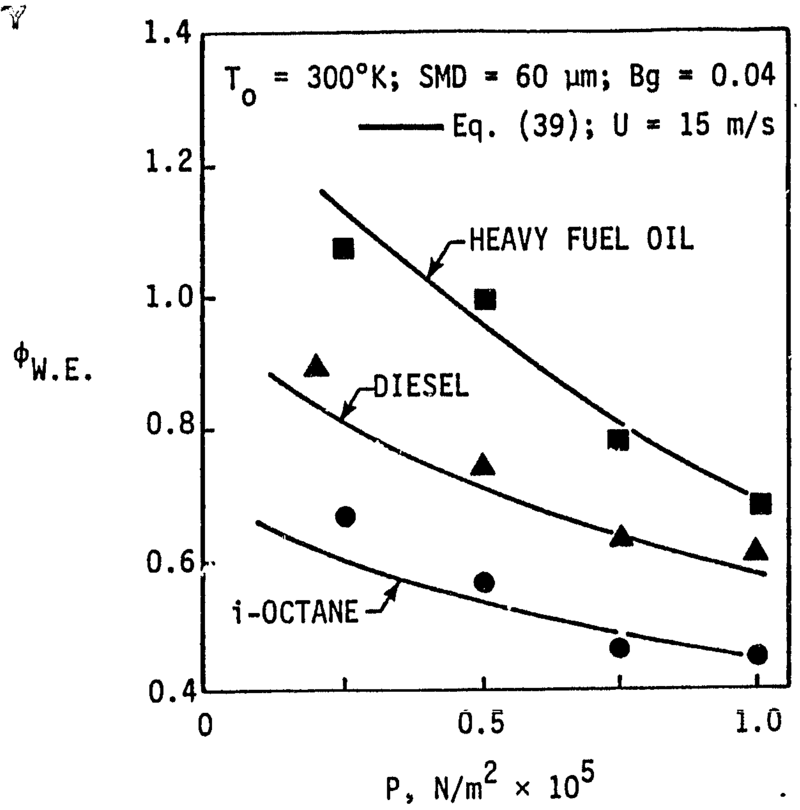


(a) Low Blockage Ratio

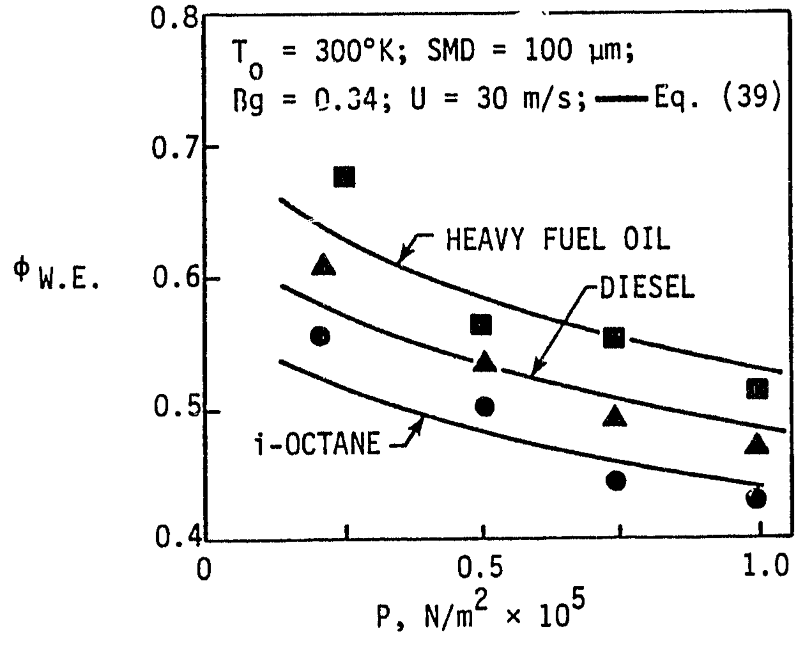


(b) High Blockage Ratio

FIGURE 14. Effects of Spray Drop Size (SMD) on Weak Extinciton Limits.



(a) Low Blockage Ratio



(b) High Blockage Ratio

FIGURE 15. Influence of Pressure on Weak Extinction Limits.

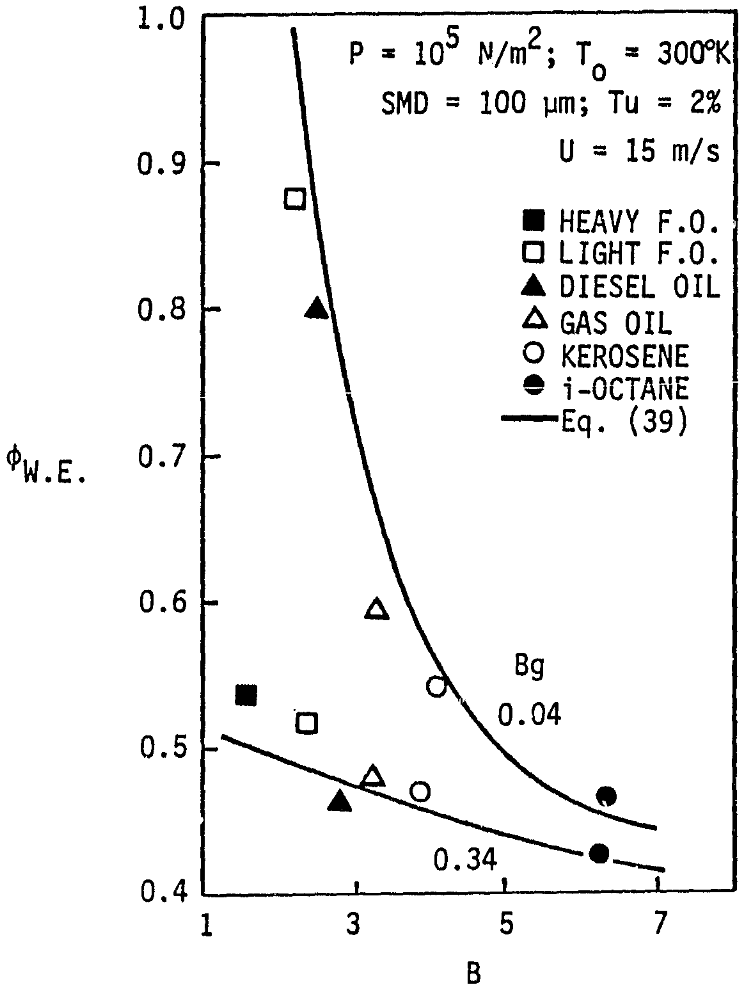


FIGURE 16. Influence of Fuel Transfer Number, B, on Weak Extinction Limits.

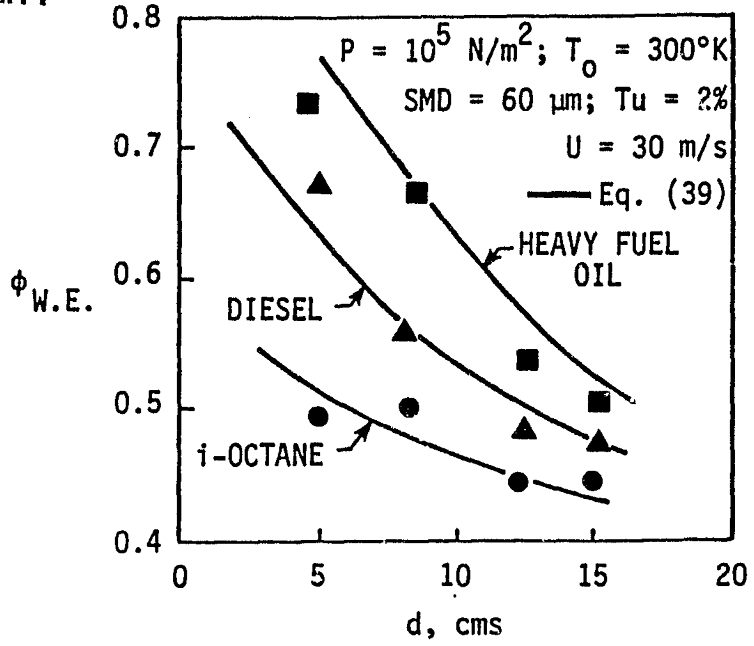


FIGURE 17. Effects of Flameholder Dimensions on Weak Extinction Limits.

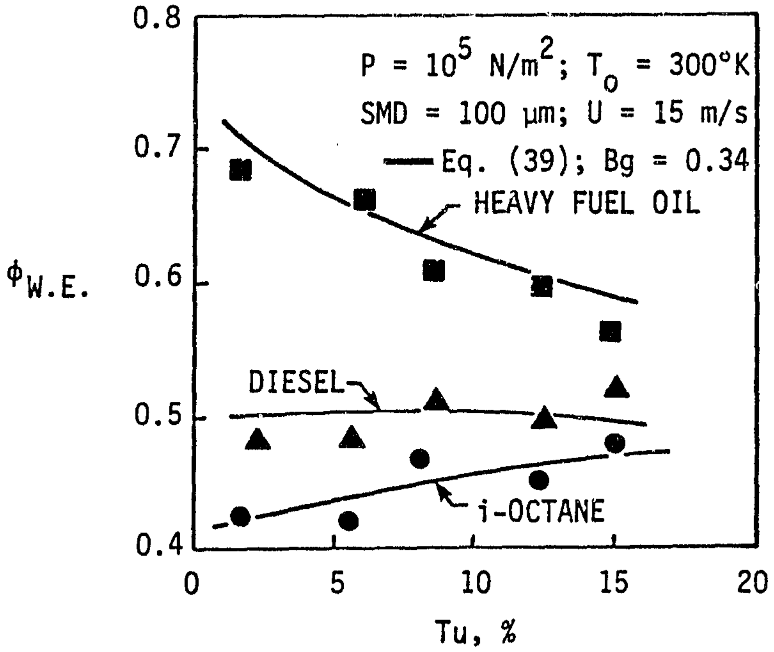


FIGURE 18. Influence of Mainstream Turbulence Intensity on Weak Extinction Limits.

increased blockage and increased turbulent intensity. In general, for the configurations and range of conditions considered, the theory predicts, and the experimental data confirm, that for heterogeneous mixtures of fuel drops and air, the weak extinction limits may be extended to lower values of equivalence ratio by increases in combustor size, fuel volatility, air pressure and temperature, and by reductions in air mass flow rate and mean drop size.

The work carried out by Ballal and Lefebvre [19] which resulted in the correlating expression given by Eq. (39) was concerned with the weak extinction limit because that limit is of interest in gas turbine operations. In a gas turbine combustor, the primary zone is operated at or near stoichiometric conditions, and lean operation is of interest from the standpoint of NO_x and soot control, with reduction of soot emissions being of overriding importance in certain applications. Industrial burners, on the other hand, operate with fuel-rich primary zones, in general; optimization of the combustion process is achieved through staging of secondary air. Thus, a need for industrial burner applications is to carry out work similar to that done by Ballal and Lefebvre, but with rich extinction as the primary focus. Again, as has been the case with much of the work discussed in this document, the need exists for conventional as well as alternative fuels.

From the standpoint of ignition and flame stabilization characteristics, the data requirements are similar to those for heterogeneous processes, with the addition of chemical kinetics data. The requirement for data related to fuel spray formation and consumption processes arises from the influence that these effects exert on ignition and flame stabilization phenomena, as outlined in this section. Chemical kinetic data needs are not explicit in the relationships outlined in this section, but are implicit in the strong temperature dependencies inherent in the flame stabilization correlations that have been discussed. These needs for chemical kinetic data will be considered from additional viewpoints in subsequent sections.

2.2.2 Flame Temperature and Laminar Flame Speed

In the discussions to this point, we have considered various mechanisms involved in the combustion process, and the impact of fuel properties on these mechanisms. Flame temperature and laminar flame speed do not represent mechanisms, but can be thought of as indicators that provide some insight into the effects of different fuels on combustion mechanisms. Flame temperature, at least in the adiabatic limit, provides a somewhat indirect measurement of the energy content of the fuel (and plays a role in establishing the conditions required for good flame stabilization characteristics, as discussed in the preceding section.) Laminar flame speed provides a measure of the reactivity of a fuel and is crucial to determining several aspects of the performance of a laminar burner (such as flashback and lift). It does not provide a directly useful performance indicator for turbulent flames, since for a turbulent flame the flame speed is much greater than, and essentially independent of, its laminar value. Laminar flame speed is useful for reaction rate determination, however.

The adiabatic flame temperature for any combustion process can be computed by applying a simple energy balance provided that the product species are known and the enthalpy-temperature relationships for all reactant and product speccies are available. Given this information, the resulting flame temperature is a function only of the initial reactant temperature and the fuel-air ratio. Enthalpy-temperature relationships are available for most product species and many fuels, but, in general, this information must be obtained for each fuel to be considered as an alternative fuel. Techniques are available for the estimation of the vapor phase heat capacity. For example, using the method of Thinh, et al. [outlined in Reid, et al., Ref. 20, pp. 228-234], vapor phase heat capacity can be obtained for a given fuel using only bond structure data; errors are estimated to be less than 5% for temperatures between the boiling point and $3000^{\circ}K$. Heat of formation and heat of combustion are then required. For a multicomponent fuel, the heat of combustion must be determined experimentally. To determine the heat of formation, the chemical formula for the fuel must be specified and then the heat of formation is estimated from the relationship

$$\Delta H_f = a\Delta H_f[CO_2(g)] + \frac{b}{2}\Delta H_f[H_2O(g)] + d\Delta H_f[SO_2(g)] + \frac{c}{2}\Delta H_f[N_2(g)] - \Delta H_c \quad (40)$$

for the arbitrary fuel molecule $C_aH_bO_cS_dN_e$ and the reaction

$$C_aH_bO_cS_dN_c + (2a + \frac{b}{2} + d - \frac{c}{2})O_2 \longrightarrow aCO_2 + \frac{b}{2}H_2O \quad \text{[illegible]}O_2 + \frac{c}{2}N_2$$

The calculation is performed at a specified reference temperature, and ΔH_f is the heat of formation, ΔH_c the measured net heat of combustion.

The second part of the information necessary involves the species existing after combustion at the final temperature. The highest temperature possible will be obtained if fully-reacted products of combustion are assumed (for stoichiometric fuel-air ratios or leaner) or a combination of fully-reacted products and unreacted fuel (for fuel-rich fuel-air ratios). However, for stoichiometric or fuel-lean combustion, dissociation is likely, and the presence of dissociated products, particularly OH, H, and CO, has a strong effect on the temperature achieved. For fuel-rich combustion, final products can include pyrolyzed fuel fragments and soot, in addition to the dissociated species already noted. One approach to determining, for a given fuel, the species present at the final temperature involves computing the adiabatic equilibrium composition for a given set of reactants. This computation requires additional information. For example, if minimization of the Gibbs free energy is the technique used to compute the equilibrium composition, data for the entropy of the species present is required.

While equilibrium species concentrations can be obtained for given fuel compositions provided the thermodynamic data are available, the computation itself involves several somewhat arbitrary decisions. Foremost among these is that the species present at equilibrium must be specified. This requires, for fuel-rich combustion, knowledge of the pyrolysis products of the fuel and their thermodynamics. Further, although a given species may be thermodynamically favored in equilibrium, the rate constant for the reaction producing that species may be so low that in practice the species would never be observed. Misleading results can in such a case be produced by an equilibrium calculation, even though the computation was correct in all other respects.

Clearly, a requirement for accurate estimation of flame temperature for an alternative fuel is a fairly detailed knowledge of both the fuel composition and its likely reaction products. Of special importance is obtaining these data for fuel-rich conditions, since it is fuel-rich equivalence ratios that are likely to be observed in the primary recirculation zones of industrial burners.

Laminar flame speed can, for a single-step reaction, be shown to be given by the simple relation

$$S_f = \left(\frac{k\dot{W}}{\rho^2 C_p}\right)^{1/2} \tag{41}$$

where k, ρ, and C_p are the gas phase thermal conductivity, density, and heat capacity of the unburned mixture. The term $\frac{\dot{W}}{\rho}$ represents the volumetric consumption rate of the fuel via the assumed single-step reaction. Eq. (41) shows that it is the gas-phase transport properties and the chemical kinetics process, taken together, that determine the laminar flame speed: in more sophisticated numerical models, a complete finite-rate kinetics mechanism and multicomponent diffusion analysis is used to compute the relation between kinetics and diffusion that defines the flame speed.

As was noted earlier, the laminar flame speed is, of itself, of little importance with respect to industrial burner applications of alternative fuels. However, given data for k, ρ, and C_p for a fuel, and a measurement of S_f obtained using a flat flame or bunsen flame apparatus, Eq. (41) can be used to estimate the different reactivities of candidate alternative fuels, so that those fuels which would need special handling because of low or high reactivity could be identified.

2.2.3 Chemical Kinetic Phenomena

The chemical kinetics of the combustion process have been implicit in much of what has been discussed in this section, but in the present subsection several phenomena that depend primarily and explicitly on chemical kinetics are discussed. These phenomena are the completion of combustion, represented by CO and HC emissions, sooting, and emissions of pollutant species such as NO_x and SO_x. The kinetics of the oxidation process, along with the residence time in the burner and the fuel-oxidizer mixing rate, define the CO and HC emissions; sooting propensity is related to these quantities and the structure of the fuel molecule, while a portion of the NO_x emissions and the SO_x emissions are related to the presence of bound nitrogen and sulfur in the fuel molecule, as well as the local temperature and fuel-air ratio spectrum in the flowfield.

CO and HC Emissions

Estimation of the CO and HC emissions produced by a given fuel in a given combustion process requires a chemical kinetics model that is sufficiently detailed to incorporate these species. Simple, one-step approaches do not incorporate sufficient detail, while multiple-step but undirectional models are normally not sufficiently general to be applied in a variety of combustion situations. On the other hand, detailed kinetics models are computationally unwieldy for simple, neat hydrocarbon fuels, and are prohibitively complex for multicomponent fuels typical of conventional fuel oils and alternative fuels. Viable approaches are thus limited to those based on the quasiglobal formulation such as currently being developed at SAI for No. 2 fuel oil and SRC-II middle distillate.

The quasiglobal kinetics model for No. 2 fuel oil and SRC-II mid-distillate is based on work carried out to model the fuel-rich combustion of aliphatic and aromatic fuel species as described in Ref. 21. This work, which involved the analysis and interpretation of well-stirred reactor data for the combustion of isooctane and toluene, resulted in the development of a multi-step subglobal mechanism including pure pyrolysis, oxidative pyrolysis, and partial oxidation, followed by a set of reversible elementary steps to completion, along with submechanisms for soot formation, soot gasification, and NO_x formation. This chain is outlined schematically in Fig. 19. The mechanism was observed to provide an excellent characterization of the combustion of isooctane, toluene, and mixtures of these two fuels, particularly in the fuel-rich regime that is critical to the analysis of industrial burners.

Application of the quasiglobal modeling techniques to predictions of the combustion characteristics of No. 2 fuel oil and SRC-II mid-distillate requires defining the aromatic and aliphatic constituents of these fuels, developing a model fuel which mimics the molecular weight and aromatic/aliphatic character of the real fuel, and defining the thermodynamic properties of the model fuel. Taking No. 2 fuel oil as an example, work currently underway at

I. PURE PYROLYSIS	$\begin{bmatrix}\text{ALIPHATICS}\\\text{AROMATICS}\end{bmatrix} \rightarrow \begin{bmatrix}C_2H_2\\CH_4\\C_2H_4\\H_2\end{bmatrix} \equiv \text{INTERMEDIATES}$
II. OXIDATIVE PYROLYSIS	$\begin{bmatrix}\text{ALIPHATICS}\\\text{AROMATICS}\end{bmatrix} + \begin{bmatrix}OH\\O_2\end{bmatrix} \rightarrow \begin{bmatrix}CH_4\\C_2H_2\\C_2H_4\end{bmatrix} + \begin{bmatrix}H_2\\C_xH_yO_z\end{bmatrix}$
III. PARTIAL OXIDATION	$\begin{bmatrix}\text{ALIPHATICS}\\\text{AROMATICS}\\CH_4\\C_2H_2\\C_2H_4\end{bmatrix} + \begin{bmatrix}O_2\\OH\end{bmatrix} \rightarrow \begin{bmatrix}H_2\\CO\\C_xH_yO_z\\CO_2\\H_2O\end{bmatrix}$
IV. ELEMENTARY STEPS TO COMPLETION	$\begin{bmatrix}CO\\H_2\\C_xH_yO_z\\H_2O_2\end{bmatrix} + \begin{bmatrix}O\\H\\OH\\CHO\\HO_2\end{bmatrix} \rightleftarrows \begin{bmatrix}H_2O\\CO_2\end{bmatrix}$
V. SOOT FORMATION	$\begin{bmatrix}\text{ALIPHATICS}\\\text{AROMATICS}\\\text{INTERMEDIATES}\end{bmatrix} \rightarrow \text{SOOT}$
VI. SOOT GASIFICATION	$\text{SOOT} + \begin{bmatrix}O_2\\CO\\CO_2\\H_2O\\H_2\\OH\end{bmatrix} \rightarrow \begin{bmatrix}CO\\CO_2\\CH_4\end{bmatrix}$
VII. NO_x FORMATION	$\text{FUEL} + \begin{Bmatrix}\text{FBN}\\N_2\end{Bmatrix} \rightarrow \begin{bmatrix}HCN\\NH_i\end{bmatrix}$ $\begin{bmatrix}HCN\\NH_i\end{bmatrix} + \begin{bmatrix}O_2\\OH\end{bmatrix} \rightleftarrows \begin{bmatrix}NO\\NO_2\end{bmatrix}$ BOUND NITROGEN AND/OR FUEL RICH NITROGEN CONVERSION $\begin{bmatrix}N_2\\O_2\\N\end{bmatrix} + \begin{bmatrix}O\\N\\OH\end{bmatrix} \rightarrow NO + \begin{bmatrix}N\\O\\H\end{bmatrix}$ THERMAL FIXATION

FIGURE 19. Generic Quasiglobal Model.

SAI [22] has shown that this fuel can be represented as a mixture of 65% dimethyl tetralin and 35% n-pentadecane. The relative amounts of aromatics and aliphatics can be determined from this representation: in the No. 2 fuel oil model cited above, the n-pentadecane constitutes the aliphatic portion of the fuel oil and the dimethyl tetralin constitutes the aromatic part.

With the model fuel and kinetics approaches both defined, the chemical kinetics model and fuel modeling can both be verified by comparison with laboratory scale experimental data. These data include well-stirred reactor measurements, of both steady-state temperature and species distribution, and blowout phenomena (at both fuel-lean and fuel-rich equivalence ratios), plug-flow ignition delay and completion of reaction experiments, and laminar flat flame and bunsen flame experiments to establish intermediate species and their concentration, as well as laminar flame speed. Thus verified, the approach can then be used to analyze a given combustion process from the standpoint of the effects of the fuel studied on the performance and emission characteristics of the burner.

The fundamental fuel data required for the development of the kinetics models necessary to evaluate completeness of combustion in a given geometry thus includes fuel composition determinations and the data required to obtain the thermodynamic properties of the fuel, as outlined in the preceding section. These data are necessary for the establishment of an appropriate chemical kinetics model: verification of the model requires that a suite of careful unit-process combustion experiments be carried out using the fuel in question. These unit-process experiments include well-stirred reactor, plug-flow reactor, and laminar flame studies; all are at laboratory bench scale, and each provides the fundamental data required to describe specific regimes of the overall reaction process. The stirred reactor provides information on post-initiation reactions relevant to flame stabilization in back-mixed primary zones. The plug-flow reactor provides information on both the initiation reactions relevant to ignition and on reactions relevant to completion of the oxidation process. Laminar flame reactors provide information on flame speed as affected by molecular transport and broaden the range of conditions covered by the other reactors.

Soot Formation

Soot formation is an area of considerable concern in industrial burner applications. One indicator of the propensity of a given fuel to form soot it its aromaticity (defined as the percentage of carbon atoms in aromatic bonds relative to the total number of carbon atoms in the fuel molecule). For example, in the work reported in Ref. 21, which was in part concerned with establishing the sooting propensity of a variety of fuels, three categories of fuels were defined, as shown in Table 10. The first group of fuels listed in the table produced large amounts of exhaust hydrocarbons in fuel-rich combustion without significant formation of soot. The second and third group produced measurable soot in fuel-rich operation, with the third group producing very much greater quantities than the first two. All of these determinations were made using a well-stirred reactor. What is significant is that both aromaticity and sooting increase progressively from Group 1 to Group 3.

TABLE 10

FUEL CLASSIFICATION BY LEVEL OF SOOT EMISSION

Group 1	Group 2	Group 3
Ethylene	Toluene	1-Methyl-Naphthalene
Hexane	O-Xylene	Other multiple ring aromatics
Cyclo-hexane	M-Xylene	
N-Octane	P-Xylene	
I-Octane	Lumene	
Cyclo-octane	Tetralin	
Decalin	Dicyclo-pentadiene	

Low hydrogen content is another consequence of high aromaticity. The atomic hydrogen to atomic carbon ratio, (H/C), one measure of hydrogen content, was shown to be an effective parameter for correlating smoke and radiation data by Naegeli [23], from measurements of aromatic doped petroleum fuels burned in a gas turbine combustor. These results are shown in Figs. 20 and 21. The sharp increase of exhaust smoke when the hydrogen/carbon ratio is reduced below two is

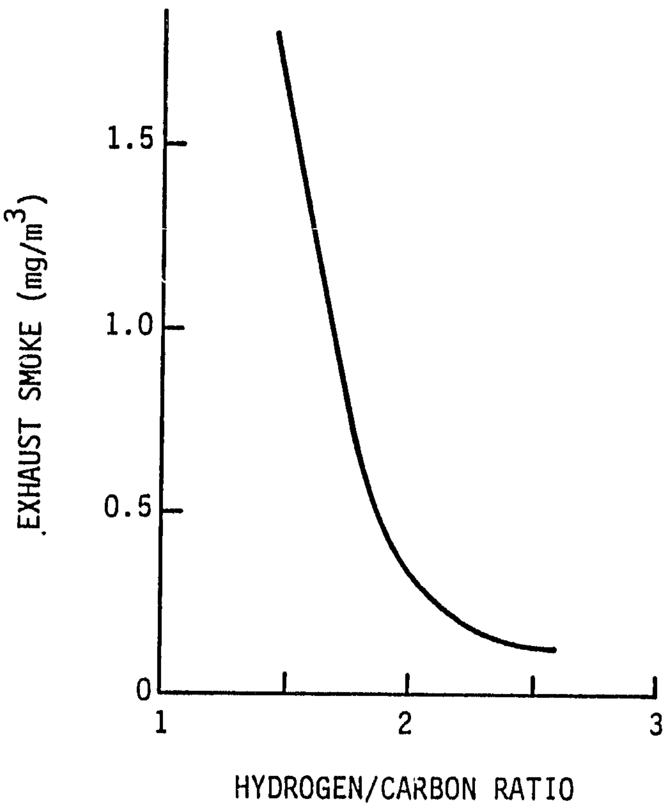


FIGURE 20. Effect of Hydrogen to Carbon Ratio on Exhaust Smoke.

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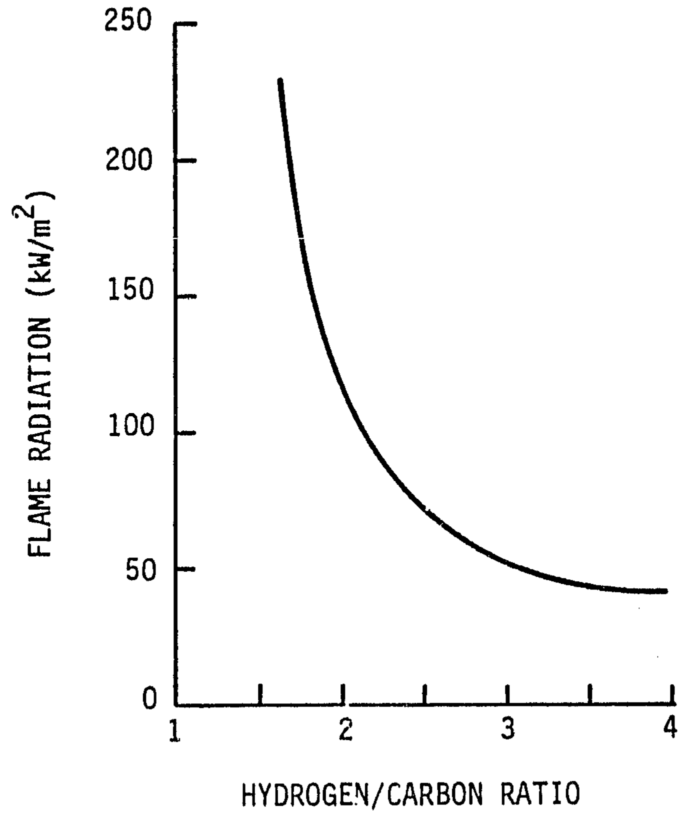

FIGURE 21. Effect of Hydrogen to Carbon Ratio on Flame Radiation.

significant because synfuels made from coal may approach hydrogen/carbon ratios of 1.2, whereas petroleum fuels exhibit an H/C ratio of about two or greater. Apart from emissions considerations, heavy sooting increases thermal radiation, decreases flame temperatures, and increases the tendency to foul equipment. Fig. 21 shows the effect of hydrogen/carbon ratio on flame radiation. The rapid increase in flame radiation below a hydrogen/carbon ratio of about two is caused by the production of soot, since soot is a continuum radiator and considerably more efficient at heat transfer by radiation than gas phase based radiation from CO_2 and H_2O. Note that the flame temperature reduction and radiation increase tend to balance so that thermal efficiency remains essentially constant. However, the distribution of heat load within the combustor may be radically altered with consequent effects on burner operation and durability.

Further evidence of the propensity of aromatic fuels to form soot is provided by the data presented by Wang [24]: these data, shown in Figs. 22 and 23, indicate that aromatics form soot more rapidly than the most prolific soot-forming straight-chain hydrocarbons, acetylene and butadiene, and form more soot the greater the aromaticity. Shock-tube data reported by Wang, Farmer, and Matula [25] and Graham [26] are shown in these figures; the soot yields were determined by laser attenuation.

There is general agreement in the literature that the overall soot formation process is triggered by hydrocarbon pyrolysis and involves subsequent soot nuclei formation, soot particle formation, and particle growth and coagulation. Recent attempts to model this process have had some success. For example, Tesner, et al. [27], proposed a model where soot formation is characterized by three rate equations. The unique feature of this model is that all the complex elementary steps associated with pyrolysis, nuclei formation and soot formation are grouped into three subglobal steps which are characterized by three separate equations. The model includes a first order (with respect to hydrocarbon concentration) pyrolysis rate, a chain branching and chain termination rate, and a soot formation rate. In contrast to this three step scheme, Kahn and Greeves [28] developed a model, using diesel engine data obtained at high pressures, which consists of a single global equation expressed in terms of local hydrocarbon concentration and local equivalence ratio. Both of

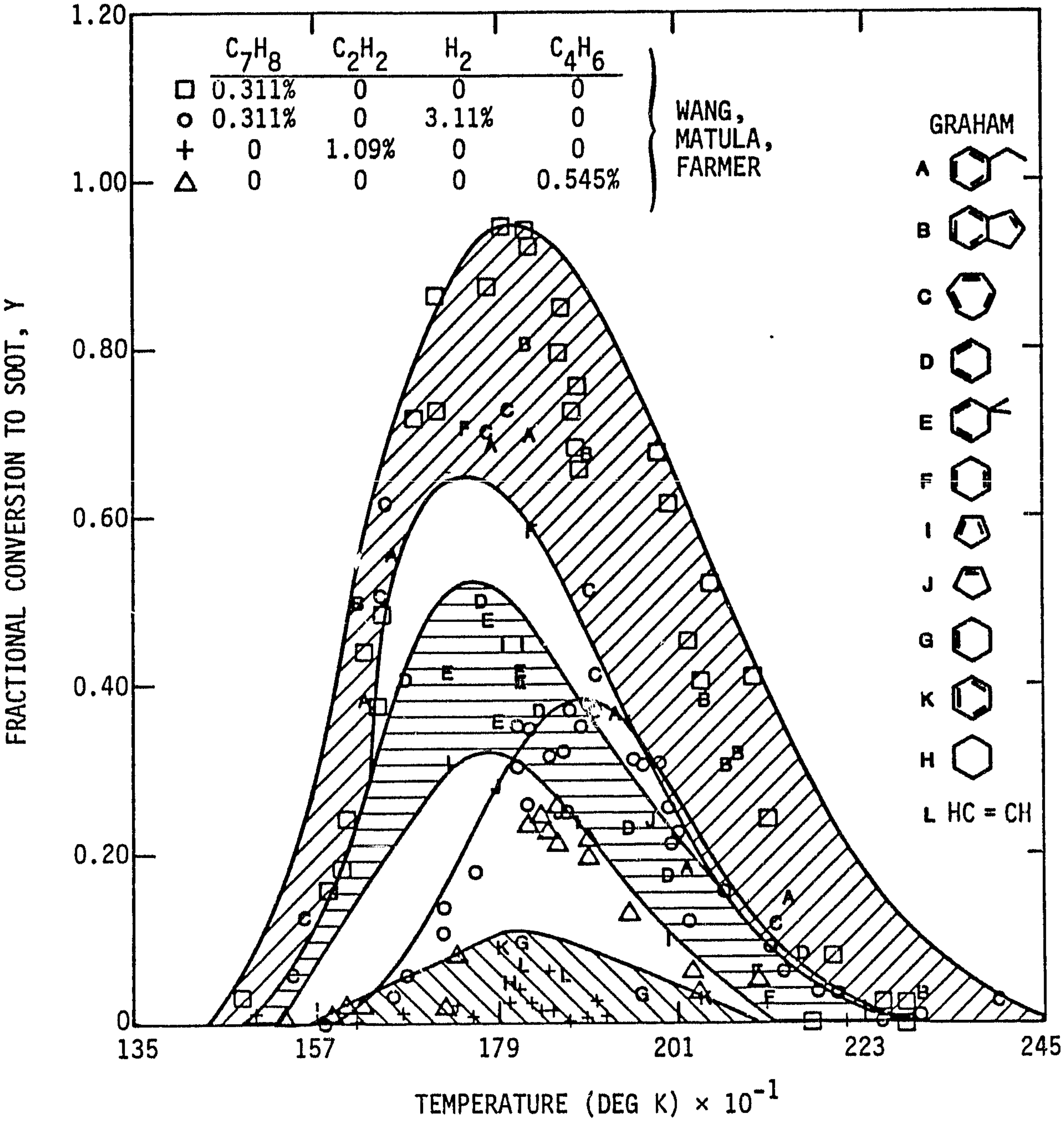

FIGURE 22. Comparison of Soot Yields at 2.5 ms After the Onset of Reflected Shocks for the Pyrolysis of Various Hydrocarbon and Argon Mixtures at Same Carbon Atom Concentration, C_5 = 2.0E+17 C atoms/ml.

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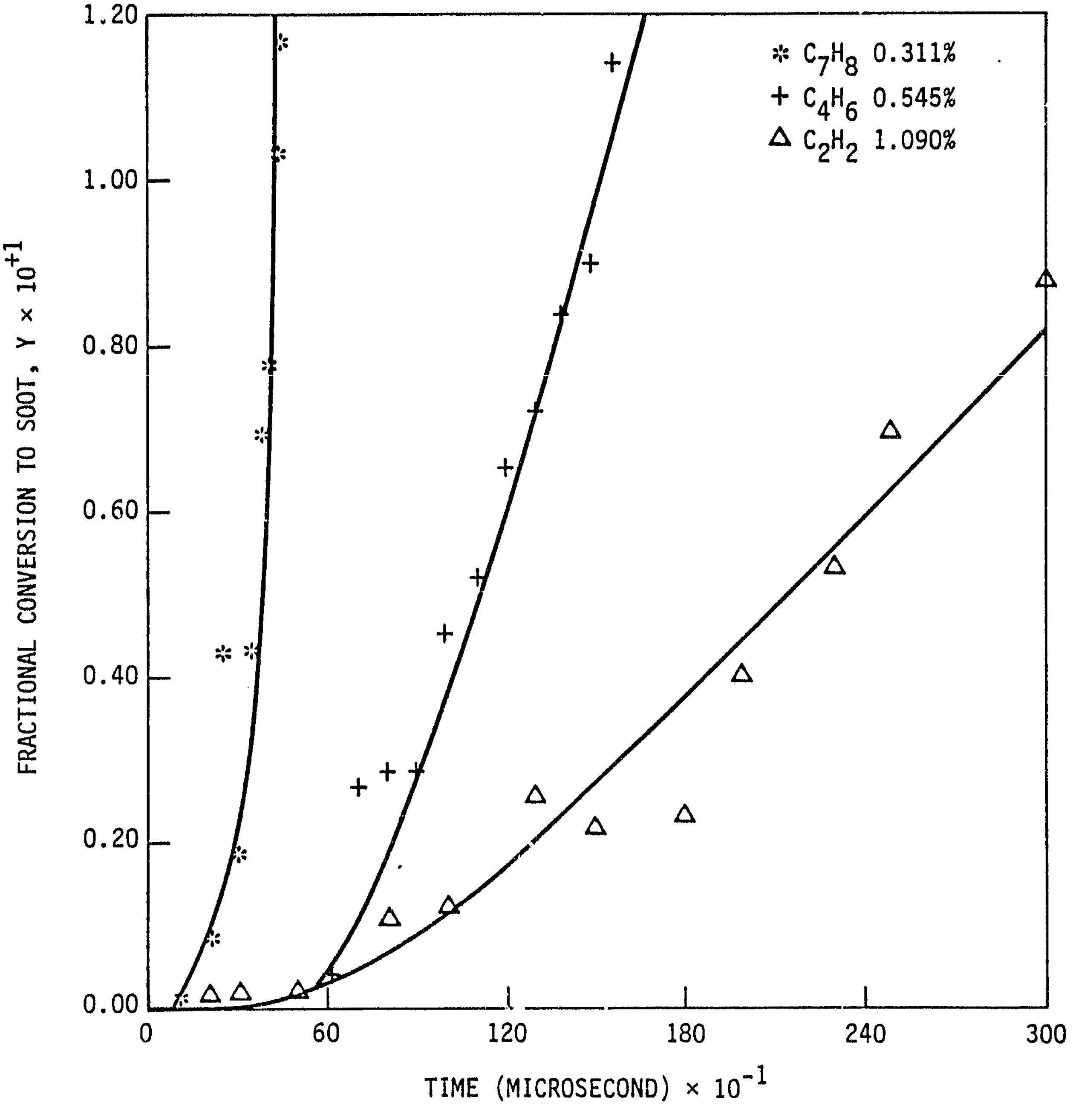

FIGURE 23. Comparison of Soot Yields During Pyrolysis of Toluene, 1,3-Butadiene and Acetylene as a Function of Time, T_5 = 1860 K, C_5 = 2.0E+17 C atoms/ml.

these approaches were evaluated by Edelman, et al. [29], and the results show that only the Kahn and Greeves model exhibits the sensitivity to inlet equivalence ratio shown by the data, but neither can adequately represent the experimental observations.

To complete the picture of soot emission in combustion systems, the effect of soot oxidation has also to be considered. Particularly in high temperature systems, soot burnout due to oxidation can be expected to be significant. Lee, Thring, and Beer [30] present a model for soot oxidation which is first order in oxygen. Other models, such as that proposed by Nagle and Strickland-Constable [31], employ a reaction order varying from zero to unity. Both of these oxygen-based oxidation kinetics formulations have been found to be reasonably reliable. However, the Nagle and Strickland-Constable model has been found to be more general because it includes more kinetic features of the surface reaction mechanism; in fact, it can be shown that the Lee et al. model is a degenerate form of the Nagle and Strickland-Constable model.

Modeling of the soot formation process is a major feature of work currently underway at SAI [22]. This modeling includes not only the chemical kinetics of soot formation but also the physical aspects, including nucleation, growth, and coagulation. The reason for this is that while the types of soot formation and oxidation models so far discussed predict the net soot yield, they do not predict the number and size of the particles. However, four parameters are required to characterize the soot phase in a flame: the soot volume fraction or mass concentration, the soot number density, the soot particle size distribution, and the mean soot particle size. Current models of the combustion process can account for the transport of soot particles, and thus provide a more accurate determination of the effects of soot on flame radiation and flame temperature, for example, than has heretofore been possible. Thus, the need to be able to model the aspects of sooting phenomena beyond net soot yield arises; this allows a more direct connection between fuel properties (which result in soot) and their effects on the combustion process in general to be made.

As was the case for the parameters which impact the completion of combustion, as outlined earlier in this section, estimation of the effects of an alternative fuel on a given combustion process through the mechanisms involved in soot formation and consumption requires a determination of the fuel composition and the data required to obtain the fuel's thermodynamic properties. Further, data is required in general (i.e., for conventional fuels as well as for alternative fuels) in order to sort out the mechanisms involved in the physical rate processes (nucleation, growth, aglommeration) that affect soot. Once again, unit process, bench-scale experiments involving well-stirred reactor, plug flow, and laminar flat flame configurations are called for, along with supporting analysis sufficiently detailed to provide tools for the investigation of the complex phenomena involved in soot formation and consumption.

NO_x and SO_x Emissions

There are two major sources of emissions of oxides of nitrogen from a combustion process: decomposition of fuel-bound nitrogen and the thermal fixation of atmospheric nitrogen. Emissions of oxides of sulfur, on the other hand, are essentially all caused by trace amounts of sulfur found in the fuel. Thus, the composition of the fuel plays a major role in both NO_x and SO_x emissions, with the thermal history of the combustion process defining the fixation of atmospheric nitrogen and the extent to which each of the rate processes involved proceed toward completion.

Thermal fixation of nitrogen is described by the extended Zeldovich mechanism

$$O + N_2 \rightleftarrows NO + N$$

$$N + O_2 \rightleftarrows NO + O$$

$$N + OH \rightleftarrows NO + H$$

for which rates are well defined and which has been supported by many studies of the NO_x formation mechanism. However, with many alternative fuels, conversion of fuel-bound nitrogen is a significant contributor to overall NO_x emissions. this is demonstrated by the data shown in Fig. 24, which are from the work reported

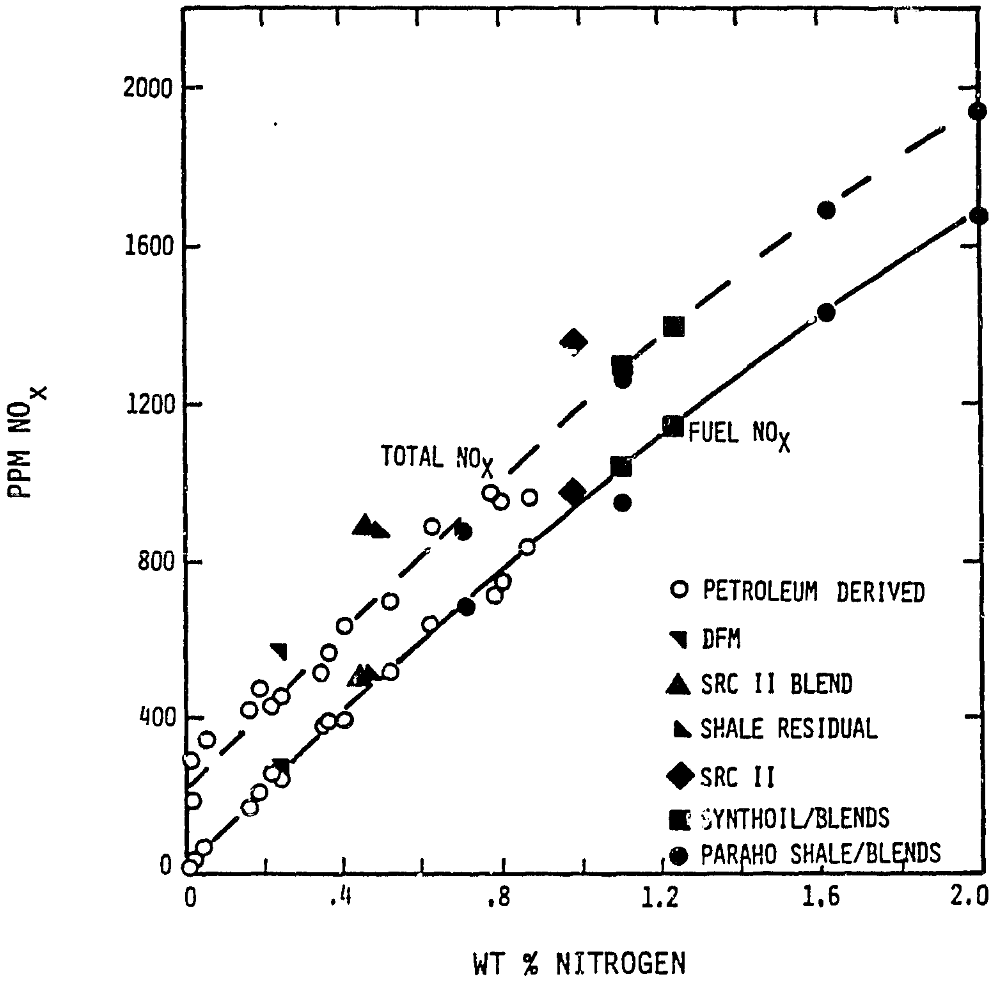

FIGURE 24. THE EFFECT OF FUEL NITROGEN CONTENT ON TOTAL AND FUEL NO_X.

in Ref. [32] and were obtained by direct substitution of the synthetic liquid fuels listed for fuel oil in oil-fired burners. Control of NO_x emissions from combustors burning alternative fuels thus requires an understanding of the processes involved in fuel-bound nitrogen conversion.

Various kinetic schemes have been proposed to describe fuel-bound nitrogen conversion. These schemes differ in detail, but the experimental observations show that regardless of the source of fuel nitrogen, only hydrogen cyanide and nitric oxide leave the primary reaction zone, while NH_x species (for example N, NH, NH_2, and NH_3) are formed subsequently in the post-flame gases. Thus, it has been postulated [33] that the fuel-bound nitrogen rapidly decomposes to HCN which then forms NO. Levy [33] proposed a set of 30 reactions to help explain the path from HCN to NO. However, little work has yet been done on the kinetics of the conversion of bound nitrogen to HCN.

The pathways involved in the formation of SO_x from fuel-bound sulfur are, like those involved in NO_x production from fuel-bound nitrogen, still a subject of research. However, hydrogen sulfide, H_2S, removed as a product during hydrodesulfurization of coal liquids, is an impurity found in some natural gases and is an intermediate species in the gasification or combustion of distillate fuels or coal-containing organic sulfur compounds. Hydrogen sulfide has received considerable attention and has been frequently doped into flames for the study of SO_x production from flames. Thus, the most widely described pathways for SO_x production initiate with H_2S contained in the fuel.

A postulated mechanism involves first a pyrolysis of H_2S producing HS, H, and free sulfur. This is postulated as an initial step since the inner part of an H_2S laden diffusion flame is rich in H_2S. HS can also be produced by OH attack on H_2S, and oxidation of H_2S by O atom. Further oxidation of HS and S then produces SO_2, and conversion of SO_2 to SO_3 proceeds by a slow third-body mechanism. In the post-flame region, as the temperature falls, both the formation and depletion rates of SO_3 will decrease as radical concentrations are decreased by recombination reactions. In fuel-rich combustion the attack of SO_3 by CO producing SO_2 and CO_2 is thought to be important [34], since SO_3 is generally absent under these conditions. However, other investigators have noted that the high level of CO produced in a staged combustion process can enhance SO_3 emissions [35], although this may only be a transient phenomenon.

Clearly, for NO_x and SO_x emissions characteristics, as well as the other chemical-kinetic related subelements considered in this section, the major data need involves measurements of the composition and thermodynamic properties of alternative fuels. For alternate fuels there is also a clear requirement for bench-scale, unit-process laboratory experiments to help delineate the kinetic pathways critical to the formation of NO_x and SO_x emissions from fuel-bound nitrogen and sulfur.

2.3 Operational and Durability Characteristics

The final group of characteristics included in Table 1 involves fuel characteristics that impact the storage and handling of fuel, and the fouling and corrosion characteristics that result from use of the fuel. While these characteristics are not of primary importance to the combustion process, they impact it in two ways: fuel additives used to ameliorate storage and handling problems can affect the fuel combustion process, and fouling and corrosion of elements of the burner and furnace can affect both the primary combustion process, through alteration of the burner aerodynamics and nozzle characteristics, and the heat transfer from the flame through coating of burner walls and heat exchanger surfaces.

The stability of liquid fuels under short- and long-term storage conditions is an area of current concern, particularly with respect to composition and physical property changes that can occur. Stability of a fuel refers to its resistance to chemical degradation that might occur as a result of thermal stress or during long-term storage. Sedimentation and deposit formation are typical manifestations of fuel instability problems. Extensive work has been done to monitor and characterize stability behavior for both synthetic and petroleum base fuels [34,35]. Since observed residues were determined to be oxides rather than polymers, it has been concluded that autoxidation is apparently the primary mechanism for initiating deposit formation; deoxygenated fuels also form deposits, but at a slower rate than fuels containing oxygen. Hetero-compounds containing nitrogen, oxygen, sulfur, and trace metals, particularly copper, are detrimental to fuel stability.

Thermal stability of aviation gas turbine fuels is characterized by the ASTM-CRC Fuel Coker and by the Jet Fuel Thermal Oxidation Tester (JFTOT). Some samples of coal-derived synfuels have been reported to have failed this test through the formation of visible deposits [35]. Accelerated storage stability tests of synfuels have also been reported [36]. In these tests, observations were made over a 32-week period for fuels held at 43.3°C, and over a 16-hour period for samples held at 93.3°C. At 43.3°C, thirteen weeks corresponds to about one year of normal storage for petroleum fuels, so that the 32-week storage period should correspond to about 2½ years of real time. However, the accelerated time/real time correlations for petroleum fuels were found not to apply to synthetic fuels, so that the amount of real storage time involved in these tests can only be considered to be approximate. The results of the thermal stability tests reported in Ref. 36 were that high gum levels were observed for the synfuels tested (Exxon Donor Solvent naphthas) especially during the latter half of the 32-week period. Viscosity did not change significantly during this period, and only slight composition changes were observed.

In general, the more highly processed the fuel, whether it be a coal-derived or a petroleum-based liquid, the better its thermal and oxidative stability. This generalization implies that specific fuels of interest should be studied since observations relative to classes of fuels could be misleading. Research on fuel stability is continuing and more fundamental studies concerning the detailed chemistry of sediments and deposits are in progress [37]. The current understanding of synfuel stability requires that stability behavior be monitored to establish exactly how important the chemical degradations associated with thermal and storage stability are with respect to overall combustion behavior.

Further data on fuel performance are given by the standardized ASTM experiments. Many of these experiments cannot be related to specific physical properties, but they do give some indication of the fuel's combustion behavior. Handling properties like pour point, flash point, and stability are included in the ASTM specifications, and fuel quality, as determined by water, sediment, metals, ash, and asphaltene content, are also covered.

3. CONCLUSIONS: SUMMARY OF COMBUSTION CHARACTERISTICS AND KEY CHEMICAL AND PHYSICAL PROPERTIES

The chemical and physical property interaction rankings given in Table 1 follow from the considerations discussed in the preceding section. Thus, Table 1, which is repeated here for convenience, serves as a summary of the material discussed in Section 2 of this report. Each physical or chemical property has been ranked in Table 1 with respect to the combustion characteristic or indicator shown in the column heading. In establishing this ranking, only primary interactions have been included. Thus, for example, the heat of combustion and heat of vaporization of a fuel affects the droplet vaporization and burninng process directly. Through the droplet vaporization phenomenon, these properties also affect ignition and flame stabilization, but this "secondary" interaction has been ignored in the summary given in Table 1. Hence, those physical and chemical properties that possess "strong" (S) or "moderate" (M) summary rankings as shown in the last column of Table 1, are properties that affect the majority of the combustion characteristics listed. However, through secondary interactions such as outlined above, certain of the apparently less important fuel properties indicated in Table 1 become of key importance also, particularly for specific combustion processes, and these will be highlighted in the discussion in this section and in the design data base development plan to be outlined in the next sections of this report.

Inspection of Table 1 shows that the chemical composition of the fuel, including hydrocarbon type and elemental and species analyses, and the chemical kinetic rates that define the consumption of the fuel are key chemical properties that impact the majority of the combustion characteristics and indicators listed in Table 1. Fuel composition is central to design that accounts for the effects of the various chemical kinetic phenomena that control the completion of combustion, sooting, and emissions characteristics. It is also central to the determination of flame temperature and laminar gas phase flame speed, as well as important in the assessement of ignition and flame stabilization phenomena. Fuel composition plays a major role in thermal and oxidative stability, as well as in fouling and corrosion. Finally, techniques for the estimation of fuel properties depend heavily on knowledge of the fuel composition.

TABLE 1. Chemical and Physical Property Interactions With Combustion Characteristics and Indicators.

GROUP	LIQUID FUEL COMBUSTION		BASIC COMBUSTION CHARACTERISTICS			CHEMICAL KINETICS			OPFRATIONAL & DURABILITY			SUMMARY
COMBUSTION CHARACTERISTIC OR INDICATOR	DROPLET AND SPRAY FORMATION ①	DROPLET VAPORIZATION AND BURNING ①	IGNITION AND FLAME STABILIZATION ①	FLAME TEMPERATURE	LAMINAR FLAME SPEED	COMBUSTION COMPLETION ①	SOOT EMISSIONS ①	NO_x AND SO_x EMISSIONS ①	THERMAL AND OXIDATIVE STABILITY	FOULING ①	CORROSION ①	OVERALL RANKING
PHYSICAL PROPERTY	DEGREE OF PROPERTY INTERACTION: STRONG (S), MODERATE (M), WEAK (W), OR NEGLIGIBLE (N)											
HEAT OF COMBUSTION, ΔH_c (OR HEAT OF FORMATION, ΔH_f)	N	S	N	S	W	N	N	N	N	N	N	W
HEAT OF VAPORIZATION, ΔH_v	N	S	N or S	W	W	N	N	N	N	N	N	W
LIQUID DENSITY, ρ_L	M	S	N or S	N	N	N	N	N	N	N	N	W
LIQUID HEAT CAPACITY, C_{P_L}	N	M	N or S	N	N	N	N	N	N	N	N	W
LIQUID VISCOSITY, μ_L	S	W	N	N	N	N	N	N	N	N	N	W
SURFACE TENSION, σ	S	W	N	N	N	N	N	N	N	N	N	N
GAS HEAT CAPACITY, C_p	N	S	S	S	S	N	W	N	N	N	N	M
GAS VISCOSITY, μ	W	S	S	W	S	N	N	N	N	N	N	W
GAS THERMAL CONDUCTIVITY, k	N	S	M	N	S	N	N	N	N	N	N	M
GAS DIFFUSIVITY, D_{ij}	N	S	M	M	S	N	N	N	N	N	N	W
VOLATILITY	N	S	M	N	N	N	N	N	N	N	N	
CHEMICAL KINETIC RATES	N	M	S	W	S	S	S	S	N	N	N	M
COMPOSITION												
• ELEMENTAL ANALYSIS	N	M	M	S	S	S	S	S	M	M	S	S
• HYDROCARBON TYPE	N	M	S	S	S	S	S	W	S	M	S	S
• SPECIES ANALYSIS	N	M	S	S	S	S	S	S	S	S	S	S
• BOUND NITROGEN	N	N	N	N	N	N	N	S	W	W	W	W
• SULFUR	N	N	N	N	N	N	N	S	M	M	M	W
• SEDIMENT	N	N	N	N	N	N	W	W	S	S	M	W
• TRACE METALS, ACIDITY	N	N	N	N	N	W	W	W	S	S	S	M

① Indicates that this combustion characteristic or indicator is strongly influenced by the flowfield aerodynamics so that a careful analytical interpretation or an unambiguous experimental definition is required to provide useful quantitative data.

Chemical kinetic rates that apply to the fuel consumption process are also crucially important to any detailed assessment of the effects of the use of an alternative fuel in an industrial combustor. This includes overall heat release reactions, critical to ignition and flame stabilization, combustion completion reactions, and those associated with soot formation and consumption and NO_x and SO_x formation. Chemical kinetic rates play a major role in the processes of ignition and flame stabilization and (along with gas phase transport properties) define the laminar gas phase flame speed.

For the other properties listed in Table 1, their criticality depends on the specific combustion process being considered, and on the secondary interactions not specifically included in the table. This can best be illustrated by reviewing each of the characteristics or indicators listed in Table 1.

Liquid Fuel Combustion

Fuel physical properties that affect droplet and spray formation processes and droplet vaporization processes are of primary importance in the liquid fuel combustion problem; thermodynamic quantities such as the heat of combustion and vaporization also play a key role. Thus, in any combustion process that involves liquid fuels, the assessment of the effects of these properties is important to the assessment of the use of an alternative fuel. Note that there are several aspects beyond those listed that must also be considered in addressing alternative fuel usage in industrial combustors. For example, the role of liquid viscosity in determining on drop size: viscosity plays a strong role in the case of pressure atomization, but for airblast atomization there is almost no fuel viscosity effect. Similarly, volatility plays a key role when the difference between the ambient temperature and the droplet boiling temperature is small, but for large values of this temperature difference (such as would be encountered with air preheat, for example) the role of volatility is much diminished. Finally, assessment of the relative effects of the physical properties relevant to the spray formation and consumption process can be carried out using suitably defined spray formation and single-droplet burning experiments in advance of specific fuel physical property data.

Gas Phase Combustion

The major gas phase combustion mechanism considered in Table 1 is ignition and flame stabilization. This process is primarily dependent on gas phase properties and chemical kinetic rates, and depends also on the thermodynamic properties of the fuel. However, the dependence on gas phase physical properties is weak for an industrial burner, in which the mixing rates that define ignition and flame stabilization characteristics are turbulent. In fact, chemical kinetic rates only begin to affect the assessment of the use of different fuels near blowout. In an industrial burner environment, much of the effect of different fuels on ignition and flame stabilization phenomena that is observed is related to the presence of fuel droplets in the flow. It should also be noted that the chemical kinetic rates that apply to the flame stabilization process in industrial burners are those for fuel-rich combustion: primary zone equivalence ratios on the order of 2 are not uncommon.

Flame temperature and laminar flame speed are two indicators of the effects of a given fuel on the combustion process, and while they may not be directly relevant to the processes which take place in an industrial burner, they provide criteria for approximating the effects that may be encountered through the use of an alternative fuel. Flame temperature is defined (at a given fuel-air ratio) by the thermodynamics of the fuel; in fuel-rich operation the fuel type, which influences the fuel decomposition pathway, also plays a role. Flame temperatures can be relatively easily defined in simple experiments and provide a useful indicator to the burner designer. Laminar flame speed, on the other hand, is not directly relevant to the turbulent combustion process in an industrial burner. However, it does serve as an indicator of the reactivity of a fuel and is thus useful to classify fuels and identify potential problems with their use. Laminar flame speed is defined by the interaction between the chemical reaction rates involved in fuel composition and the gas phase transport properties, but rather than use of these properties to determine a laminar flame speed analytically, laminar flame experiments which determine the flame speed can be used, with appropriate analysis, to determine chemical reaction rate information.

Chemical Kinetics

Analyses of those phenomena grouped together under the chemical kinetics heading are all dependent on fuel composition and chemical kinetics rate determinations. Soot, NO_x, and SO_x emissions phenomena are particularly related to fuel composition, since sooting tendency has been linked directly to fuel type (with aromatic fuels having a much greater propensity to soot than aliphatic), NO_x to the presence of bound nitrogen in the fuel, and SO_x to the presence of sulfur in the fuel. All of these processes are, in general, rate limited, however, so that kinetics data are also directly relevant: equilibrium assumptions can produce very misleading estimates of soot, NO_x, and SO_x emissions. There are a number of interactions between the completion of combustion and emissions reactions and the other aspects of the combustion process that lead to secondary relationships with other fuel properties. For example, the adiabatic flame temperature has been linked to sooting propensity, and thermal NO_x production is itself strongly dependent on temperature. All chemical kinetic processes exhibit some degree of temperature dependence so that each of the processes considered in this section is dependent on the local temperature and thus on the thermodynamic properties of the fuel.

Operational and Durability

The characteristics involved in the operational and durability group themselves have only a secondary effect on the combustion process, but can have a greater impact on the overall suitability of a fuel for a given industrial burner application. Thermal and oxidative stability, for example, refers to the tendency exhibited by some multicomponent fuels to undergo irreversible changes in species composition and certain physical properties during storage. While not completely understood, the mechanisms which lead to these problems are dependent on the composition of the fuel and, in particular, the trace metal content and acidity of the fuel. Fouling and corrosion characteristics also are defined by the fuel composition. It might also be noted, from Table 1, that the fuel property characteristics that impact operational and durability considerations (in particular sediment and trace metals content) also affect emissions characteristics of the fuel.

What this review demonstrates is that fuel composition is a basic requirement for any serious attempt at fuel combustion characteristics determination. This applies as well to conventional fuels, and the lack of detailed determination of the fuel composition in most combustion experiments has introduced a needless and unquantifiable uncertainty into the analysis of the experimental results. Fuel composition determination should be required data produced as part of any investigation of combustion characteristics. This need is particularly acute with respect to multicomponent liquid fuels whose composition can change during a test series because of evaporation or the thermal and oxidative instability processes already noted.

A second major requirement for a fuels effects data base is knowledge of the chemical kinetic rates that apply to the fuel combustion, and, when fuel-rich operation is considered, fuel decomposition processes. This rate information is central to any detailed analysis of combustion processes and, indeed, to the interpretation of combustion process experiments. Other key data required involves the gas phase physical properties, thermodynamic data, and liquid phase physical properties. These data are relevant to specific combustion processes, and their importance depends to some extent on the influence of the specific combustion process in a given industrial burner configuration. Nevertheless, in a generalized alternative fuels data base, data on gas and liquid phase physical properties and fuel thermodynamic properties should be included.

4. CONCLUSIONS: SUMMARY OF CURRENTLY AVAILABLE FUEL PROPERTY DATA BASES

There currently exist a variety of different sources for the fuel physical and chemical property data indicated as required in the preceding sections. At the present time, the collection and assessment of these data for alternative fuels has not been done, although some work in this area has been and is currently underway (see, for example, Refs. 38, 39, and 40 for synthetic liquid fuels and Ref. 41 for synthetic gases). These tabulations and others are incorporated in the annotated bibliography included as Appendix B of this report. Further, properties of compounds found in liquid petroleum-derived and alternative fuels are reported in Refs. 42 and 43, with the work reported in Ref. 42 representing continuing studies being carried out under the direction of the American Petroleum Institute at Texas A&M University (API Project 44). The American Petroleum Institute publishes a continuing series of monographs on the properties of compounds found in both petroleum-basedand synthetic fuels, of which Refs. 44 and 45 are examples. Finally, there are a number of abstracting sources which specialize in listing reports and other publications relating to fuel properties and fuel combustion characteristic information. Examples of these sources are the Navy Synthetic Fuels Reference File [46], the data base reported in Ref. 40, and the McGraw-Hill Synfuels Handbook [47].

As noted above, a critical assessment of all of the available fuel property data bases has not yet been performed for alternate fuels. Thus, the available data can be expected to be fragmentary and incomplete, particularly with respect to critical variations in fuel properties with temperature. Therefore, a key first step in the implementation of the alternative fuels design data base development plan outlined in the next section of this report must be the assessment of existing fuels property data information. This would require the assembly, from the sources outlined in the preceding paragraph and in the annotated bibliography, Appendix B, of available fuels property data. An assessment of these data would involve comparison of data for similar propoerties from different sources, estimation of data accuracy, and, where possible, comparison of the measured data with results computed using available estimation techniques [20] and fuel composition data. To aid in the assembly of available data, questionnaires have been developed as part of the current work for circulation to laboratories that are currently involved in alternative fuels research or which have been involved in such research in the past. These questionnaires are incorporated in Appendix C of this report.

5. RECOMMENDATIONS: A SUGGESTED PLAN FOR DEVELOPING AN ALTERNATIVE FUELS DESIGN DATA BASE

From the discussion of the interaction of fuel physical properties with combustion characteristics given in Section 2, and the ranking of the importance of fuel physical properties and their interaction with combustion characteristics in Section 3, a suite of specific experiments designed to develop an alternative fuels design data base can be defined. These experiments are detailed in Table 11.

The specific combustion experiments outlined in Table 11 encompass unit-process experiments (plug flow and well-stirred reactor; flat flame and diffusion flame; droplet consumption; spray characterization); experiments designed to introduce in a simplified form the effects of aerodynamic modifications to the combustion process that might be utilized in an industrial burner design (well-stirred reactor/plug flow with distributed injection; spray vaporization/burning in uniform flow), and experiments designed to provide data on the coupling of all of the mechanisms discussed in this report within the context of a model of a realistic industrial burner flowfield. This suite of combustion experiments, and the associated analysis of the experimental results would provide a comprehensive design data base on alternative fuels use in industrial combustors.

Table 11 includes the specific output from each class of experiment, the rationale for this particular experiment, and outlines the fuel property data that is required to properly interpret the experimental data. Finally, since the analysis and interpretation of experimental combustion data requires the use of analytical techniques, as does the scaling of given experimental results to apply to conditions beyond those measured or at sizes different from those considered in the experiments, the required analytical models for each type of experiment are shown in the last column.

For most of the combustion experiments listed in Table 11, fuel physical and thermodynamic property data are required to properly analyze and interpret the data, so that a major aspect of the initial phase of the suggested data base development work is the compilation of the physical and thermodynamic properties of the fuel, as shown in Table 12. This work also incorporates

TABLE 11. Combustion Experiments for Alternative Fuels Effects Determination.

EXPERIMENT TYPE	EXPERIMENT OUTPUT	RATIONALE	FUEL PROPERTY DATA REQUIRED FOR INTERPRETATION	MODELS REQUIRED FOR INTERPRETATION/SCALING
1. PLUG FLOW REACTOR ● GAS PHASE FUEL OR PREVAPORIZED; PREMIXED.	Species and temperature as function of time, inlet temperature, fuel/air ratio, pressure, heat loss. Ignition delay time. Intermediate species, NO_x, SO_x, soot. Combustion completion time.	Kinetics data; ignition data. Determine key intermediates, relationship between intermediates and NO_x, SO_x, soot. CO/HC emissions data.	Fuel composition. Fuel thermodynamic properties.	One-dimensional plug flow analysis. Finite-rate chemical kinetics formulation.
2. WELL-STIRRED REACTOR (a) GAS PHASE FUEL OR PREVAPORIZED, PREMIXED.	Species as function of residence time, inlet temperature, fuel/air ratio, pressure, heat loss. Emissions characteristics-NO_x, SO_x, soot. Blowout limits.	Kinetics data, emissions characterization, soot limits, combustion stability limits.	Fuel composition. Fuel thermodynamic properties.	Well-stirred reactor analysis. Finite-rate chemical kinetics formulation.
(b) LIQUID PHASE FUEL	As above, as function of spray quality.	Effect of liquid fuel properties on emissions, sooting, combustion stability.	As above, with liquid fuel properties, spray characteristics.	Multiphase well-stirred reactor analysis. Finite-rate chemical kinetics formulation. Droplet vaporization/burning model. Residence-time distribution function model.
3. LAMINAR & TURBULENT FLAMES ● GAS PHASE FUEL OR PREMIXED. (a) FLAT FLAME, PREMIXED.	Flame speed, species and temperature histories. Intermediate species, NO_x, SO_x, soot, as function of inlet fuel/air ratio, temperature, heat loss.	Reactivity determination, relative to fuel type, fuel/air ratio, temperature. Data for kinetics model development. Interaction of chemical kinetics with laminar and turbulent flowfield, transport properties. Effects of transport property variation. Ignition/stabilization limits.	Fuel composition. Fuel thermodynamic properties. Gas-phase transport properties. Effective emissivities for gas phase, soot.	Laminar flat flame model, with effects of diffusion, chemical kinetics, variable transport properties. Radiation heat loss model.
(b) DIFFUSION FLAME ● PARTIALLY PREMIXED AND PURE DIFFUSION.	As above.	As above.		Laminar bunsen flame model, parabolic steady-state and elliptic time-dependent, with effects of diffusion, chemical kinetics, radiation heat loss.
4. SINGLE DROPLET COMBUSTION (a) OPTICAL MEASUREMENTS.	Drop diameter as a function of time, ambient temperature, fuel type.	Burning rate coefficient and transfer number determination.	Fuel type.	Classical single drop model.
(b) DETAILED MEASUREMENTS.	As above, with detailed measure of species evolved in vaporization, burning of drop. Pyrolysis of droplet. Formation of cenospheres. Drop temperature as function of time.	As above. Investigate fuel pyrolysis, formation of cenospheres as function of fuel type, ambient environment. Data for detailed drop combustion model. Kinetics of fuel decomposition.	Fuel composition, thermodynamic properties, liquid-phase physical properties.	Detailed nonuniform temperature multicomponent fuel droplet combustion model. Finite-rate kinetics formulation.

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TABLE 11. Combustion Experiments for Alternative Fuels Effects Determination (continued).

EXPERIMENT TYPE	EXPERIMENT OUTPUT	RATIONALE	FUEL PROPERTY DATA REQUIRED FOR INTERPRETATION	MODELS REQUIRED FOR INTERPRETATION/SCALING
5. COMBINED WSR/PLUG FLOW WITH DISTRIBUTED INJECTION (a) GAS PHASE FUEL OR PREVAPORIZED.	Exit species as function of residence time, inlet temperature, fuel/air ratio, primary/secondary air injection rate, heat exchange in plug flow.	Examine in controlled simulation effects of aerodynamics and staging in combustion process as a function of fuel type. Determine techniques for minimizing NO_x, SO_x, soot. Investigate quenching effects.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data.	Coupled well-stirred reactor/plug flow with distributed injection in plug flow. Finite-rate chemical kinetics.
(b) LIQUID PHASE FUEL	As above, as function of fuel liquid properties, fuel type.	As above. Examine effects of air preheat on combustion process for liquid fuels.	As above, with liquid fuel properties, spray characterization.	Multiphase well-stirred reactor/plug flow with distributed injection model. Finite-rate chemical kinetics, droplet combustion model.
6. SPRAY CHARACTERIZATION	Droplet size, distribution as function of injector type, fuel type, fuel temperature, pressure, primary and secondary air flow rate.	Determine influence of fuel properties on spray droplet size and droplet distribution function. Investigate interaction of spray injector, fuel type, and airflow velocity as affects drop size.	Fuel liquid-phase physical properties.	Spray formation analysis - numerical or semiempirical.
7. SPRAY VAPORIZATION/ BURNING - UNIFORM FLOW	Combustion characteristics - species profiles, SO_x, NO_x, soot; temperature as function of fuel spray quality, air temperature, heat transfer rates; simplified aerodynamics.	Determine overall effects of fuel properties on combustion processes in simplified model burner simulation. Investigate effects of air preheat, staging, for spray fuel injection.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data. Effective thermal emissivity. Fuel liquid properties. Spray characterization.	Spray transport/vaporization/burning analytical model. Coupled finite-rate chemistry; single droplet and spray burning models.
8. ALTERNATIVE FUELS COMBUSTION IN A MODEL BURNER (a) GAS PHASE FUEL OR PREVAPORIZED.	Combustion characteristics - species profiles, NO_x, SO_x, soot, temperature as function of fuel type, fuel/air ratio, air temperature, heat transfer rates, representative burner aerodynamics: large scale recirculation zones, swirl.	Determine overall effects of alternative fuels on combustion processes in aerodynamics representative of industrial burners.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data. Effective thermal emissivity.	Industrial burner combustion model: turbulent mixing, recirculation zones, swirl, coupled finite-rate chemistry.
(b) LIQUID PHASE FUEL	As above, with addition of spray quality as a parameter.	As above, with addition of spray injection representative of industrial liquid-fuel burners.	As above, with addition of: Fuel liquid properties. Spray characterization.	Multiphase industrial burner combustion model; add spray transport to above specification.

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TABLE 12

SUGGESTED DATA BASE DEVELOPMENT PLAN BY PHASE AND TASK

PHASE	TASKS	OUTPUT
Basic Data Generation	Thermodynamic properties compilation Fuel composition data compilation Chemical kinetic rate determination Single droplet combustion Fuel liquid properties compilation Spray characterization	Basic composition, physical and thermodynamic property data compilation Droplet burning rate data Drop size/distribution data
Preliminary Properties Effects Determination	Multiphase well-stirred reactor experiments Single droplet combustion (detailed data) Well-stirred reactor/plug flow experiments (gas phase and multiphase)	Effects of fuel properties on the combustion process simplified systems
Alternative Fuel Effects in Industrial Burners	Well-stirred reactor/plug flow experiments (gas phase, multiphase) Spray vaporization and burning in uniform flow Model industrial burner experiments	Effects of fuel properties on the combustion process in realistic systems.

compilation of fuel composition data, for with appropriate composition data it is possible to estimate fuel properties where measured properties are not available. These estimated fuel properties can then be used in the analysis of the combustion experiments listed in Table 11, and the results of this analysis will, in turn, indicate the sensitivity of the particular combustion process to the estimated property value. This iterative procedure will allow the definition of those fuel properties for which estimated values are insufficiently accurate. More accurate values obtained by experimental measurement could then be obtained and used for further data analysis.

The basic data generation phase of the suggested program includes the stirred reactor and plug flow combustion experiments, single droplet combustion experiments, spray characterization experiments, and liquid properties data compilation work in addition to the composition, thermodynamic, and physical properties data compilations already discussed. These basic experiments would provide the data, including chemical kinetic and liquid burning rate information, and spray droplet size and distribution, necessary to provide at least a preliminary assessment of the effects of alternative fuels on combustion processes relevant to industrial burner design.

To obtain more refined estimates of alternative fuels effects on the combustion processes relevant to industrial burner design, the work outlined under the preliminary properties effects determination phase would be carried out. Because a primary impact of alternate fuels with respect to industrial burners is anticipated to involve liquid fuel combustion processes, this phase incorporates multiphase well-stirred reactor experiments (which require the spray characterization work carried out in the preceding phase for their analysis and interpretation) and more detailed single droplet experiments. For both gas phase alternative fuels and liquid fuels, the well-stirred reactor-plug flow experiments would provide an initial data base on the effects of aerodynamics, staging, inlet air heating, and other emissions control efficiency improvement techniques on the combustion process. Thus, the overall output of this phase would be an initial evaluation of the effects of fuel properties on the combustion process in simplified systems that incorporate some of the important features of industrial burners. Note that the properties data base, kinetics data base, and liquid fuel combustion processes data base obtained in the initial phase of the suggested program are all necessary for the evaluation of the data obtained during this phase.

The the third phase of the suggested program would be designed to provide a comprehensive quantification of the effects of the use of alternative fuels in industrial burners. This phase, as shown in Table 12, incorporates additional well-stirred reactor/plug flow reactor experiments, experimental investigations of spray combustion in a uniform flow, and experiments in a configuration designed to model the flowfield in a representative industrial burner. The output of this phase is then a description of the effects of fuel properties on the combustion process in realistic systems. Taken together, the suggested program will thus provide a complete and comprehensive evaluation of the impact of the use of alternative fuels on industrial burner design.

Each of the experimental efforts outlined in Table 11 interacts to some extent with the other tasks of the suggested work, as is noted in the column entitled "Fuel property data required for interpretation" in Table 11. Because of these interactions, certain of the tasks must follow the availability of data from other tasks, as is depicted in the phase/task/time interaction diagram, Fig. 25. As is shown in this figure, the initial tasks involve thermodynamic and physical properties compilation and composition data compilation, as well as single-droplet burning rate determination. This is not meant to imply that no other work can be initiated until the properties data compilation is completed, since as outlined above, certain physical and chemical properties of the fuel may be adequately estimated. Further, for many alternative fuels of interest an initial data base encompassing thermodynamic and physical properties, as well as single-droplet burning rate data already exists. Thus, although not shown in Fig. 25 explicitly, a concurrent assessment of available data should be carried out with this phase of the suggested program.

As the interactions shown on Fig. 25 suggest, there is a considerable degree of relationship between each of the tasks shown. This figure does not indicate a feedback of information between tasks, but such a feedback is a basic requirement for any well-constructed program and would be anticipated in any program structured along the lines suggested in this report.

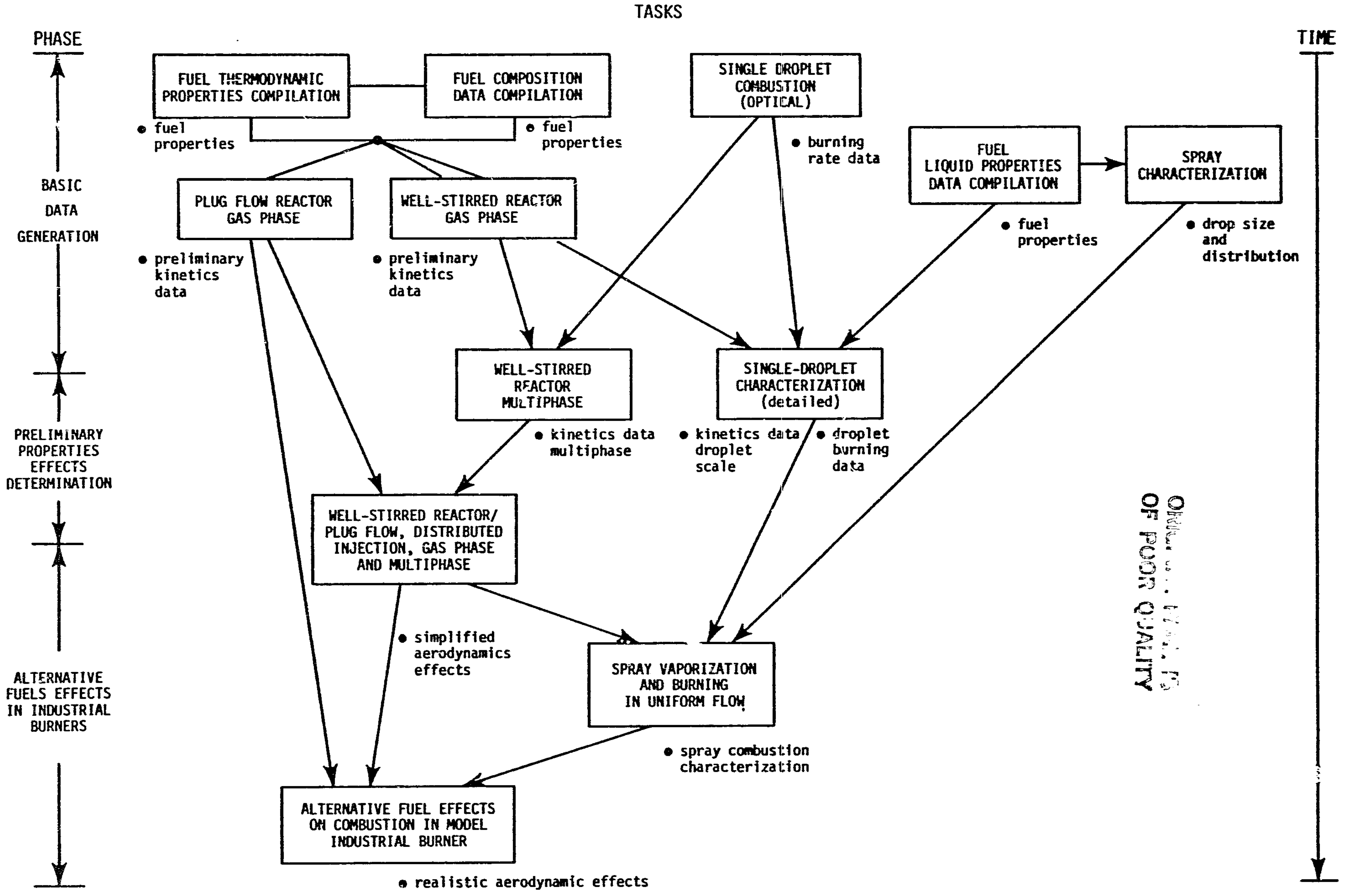

FIGURE 25. Phase-Task-Time Interaction Diagram - Alternative Fuels Effects Determination.

6. NEW TECHNOLOGY

No reportable items of new technology have been developed as part of the work reported in this document.

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APPENDIX A

FUEL PROPERTY DATA AND DATA FORMAT

As noted in the text of this report, accurate fuel composition, thermodynamic, and physical properties data is required for alternate fuels in order to assess the impact of the utilization of these fuels on industrial burner design. Assessment of the composition and properties of SRC-II mid-distillate and heavy distillate, and No. 2 and No. 6 fuel oil, is a portion o the effort being carried out in a current Department of Energy sponsored program at SAI [A1]. This work has involved both compilation of available experimental property data and estimation of these quantities where experimental data were not available. The estimation techniques used are described in Ref. A1. Some of the results of this current work are presented in this appendix as an example of data needs and data format for reporting this information.

A comprehensive summary of the property data for SRC-II MD, SRC-II HD, No. 2 fuel oil and No. 6 fuel oil is presented in Table A1. Where data have been estimated, the symbol (E) is used. It should be noted that the estimates shown in Table A1 are based on preliminary composition data and can be refined as more specific composition data becomes available. The data in this table show that SRC-II MD and No. 2 fuel oil have similar properties except for the C/H ratio and the oxygen and nitrogen content: these differences can be expected to affect the chemical kinetic behavior primarily, and could lead to greater soot and NO_x emissions from SRC-II MD than from No. 2 fuel oil.

Measured data are available for all properties except the surface tension and liquid heat capacity of No. 6 fuel oil, the heat of vaporization for all the fuels considered, the gas phase properties of each fuel, and the standard entropy of formation of these fuels. Reasonable estimates of these properties can be made using the techniques described in Ref. A1, but experimental verification of the estimated values should be carried out, especially with respect to the gas phase transport properties.

Although the data shown in Table A1 are available or can be estimated, no information is incorporated on temperature variation of the physical properties listed. This is a major difficulty: while the data available do allow

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TABLE A1. Fuel Property Data and Data Format.

	SRC-II MD	SRC-II HD	NO. 2 FUEL OIL	NO. 6 FUEL OIL
ELEMENTAL COMPOSITION				
C (WT %)	84.59	88.98	86.4	87.2
H	8.84	7.64	13.3	11.96
N	0.85	1.03	0	0.46
S	0.20	0.39	0.3	0.47
O	5.43	1.9	0	0.86
ASH	0.002	0.058	0.001	0.008
HYDROCARBON TYPES-ASTM D1319 & D2789				
SATURATES				
• STRAIGHT CHAIN	0		70.5	
• BRANCHED CHAIN	0		7.5	
• CYCLIC ALKANES	35			
OLEFINS	0		0	
AROMATICS-ASTM D1319	65		22	
SPECIES:	CRESOL XYLENOL METHYLNAPHTHALENE DIMETHYLNAPHTHALENE NAPHTHALENE TRIMETHYLPHENOL TETRALIN PHENOL METHYLTETRALIN OTHERS	ANTHRACENE PYRENE METHYLANTHRACENE METHYLPYRENE DIMETHYLBIPHENYL TRIMETHYLBIPHENYL METHYLBIPHENYL FLUORINE DIMETHYLPYRENE OTHERS	C_{12}-C_{17} N-PARAFFINS TRIMETHYLDODECANE METHYLINDAN TETRALIN METHYLTETRALIN METHYLACENAPHTHENE TETRAETHYLBENZENE METHYLPROPYLBENZENE METHYLNAPHTHALENE DIMETHYLNAPHTHALENE OTHERS	C_{18}-C_{43} N-PARAFFINS CYCLIC ALKANES AND POLYAROMATICS C_{18}-C_{53}
MEAN MOLECULAR FORMULA	$C_{12}H_{15}O_{0.6}N_{0.1}S_{0.01}$	$C_{14}H_{12.4}O_{0.2}N_{0.1}S_{0.02}$	$C_{13}H_{22}S_{0.02}$	$C_{22.8}H_{37.6}N_{0.10}S_{0.05}O_{0.17}$
MEAN MOLECULAR WEIGHT-ASTM D2503	169	185	178	315
DENSITY (g/cm^3)-ASTM D287				
@ 288°K	0.974	1.09	0.844	0.915
KINEMATIC VISCOSITY (cm^3/s)-ASTM D445				
@ 333.3°K	0.0306	0.121	0.0350	0.29
@ 371.9°K	0.0134	0.0473	0.0149	
SURFACE TENSION (dynes/cm)				
@ 295°K	33	28.5	29.9	37.3 (E)†
LIQUID HEAT CAPACITY (cal/g °K)				
@ 394°K	0.55	0.41	0.53	0.53 (E)†
HEAT OF COMBUSTION (LOWER HEATING VALUE) (Kcal/g) ASTM D240	8.994	9.122	10.161	9.88

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TABLE A1. Fuel Property Data and Data Format (continued).

	SRC-II MD	SRC-II HD	NO. 2 FUEL OIL	NO. 6 FUEL OIL
HEAT OF VAPORIZATION @ MEAN BOILING POINT (cal/g) (E)	64.2 (E)	70.3 (E)	61.5 (E)	48.3 (E)†
DISTILLATION DATA @ 1 atm (°K)				
IBP - ASTM D86	473	563	472	506
10% (Vol)	481	580	490	589
30%	492	598	515	644
50%	502	620	533	700
70%	512	652	554	756
90%	533	700	584	867
HEAT CAPACITY OF GAS 650°K (cal/g °K) (E)	0.564	0.465	0.663	0.64†
VISCOSITY OF GAS 650°K (g/cm sec) (E)	1.17×10^{-4}	1.22×10^{-4}	1.15×10^{-4}	1.27×10^{-4}†
THERMAL CONDUCTIVITY OF GAS 650°K (cal/sec cm °K)	6.38×10^{-5} (E)	6.84×10^{-5} (E)	8.81×10^{-5} (E)	9.32×10^{-5}† (E)
DIFFUSIVITY (cm²/sec) (E) D_{fuel, N_2}	2.03×10^{-1}	1.60×10^{-1}	2.02×10^{-1}	1.75×10^{-1}†
ΔS_F (cal/mol · K) (E)	120.84	107.34	140.15	†
TEST PROCEDURE				
POUR POINT (°K) ASTM D97	230.2	280.2	252.4	300
FLASH POINT (°K) ASTM D93	358	441	345	473
LUMINOMETER NO. ASTM D1740	2.0	-	29.0	
SMOKE POINT ASTM D1322	8.0	-	16.0	
WATER CONTENT (% WT) ASTM D1796	0.1 - 0.6	1.48	0	0.07
SEDIMENT CONTENT (% WT) ASTM D1796 & D473	0 - 0.05	0.02	0	0.052
METALS CONTENT (PPM WT)	(FOR A BLEND OF MD & HD)			
	TITANIUM 0.5	VANADIUM 0.23	0	
	SODIUM 1.4	LEAD 0.12		
ASPHALTENES (% WT)	POTASSIUM 1.5	IRON 13	0	1.3 - 5.0
	CALCIUM 1.6	PHOSPHORUS < 0.01		
ASH (% WT)- ASTM D482	0.002	0.028	< 0.001	0.02
EXISTENT GUM (mg/100 ml)-ASTM 2274 & D381	0.8	0	0.9, 10.7	

†ESTIMATED VALUES FOR NO. 6 FUEL OIL WERE MADE WITH THE CHARACTERIZATION FACTOR METHOD. CORRELATIONS FOR ΔS_F ARE NOT AVAILABLE USING THIS METHOD.

(E) = ESTIMATED VALUES.

first-order estimates of some of the effects of alternative fuels such as listed in Table A1 on industrial burner design to be made, more reliable estimates, as noted in Section 2 of this report, require the temperature variation information. Thus, the data shown in Table A1, while it establishes a useful baseline, does not provide the complete suite of data required to fully assess alternative fuels effects on burner design.

APPENDIX B

ANNOTATED BIBLIOGRAPHY

The reports, papers, books, and conference or symposium proceedings listed in this appendix provide a variety of sources of alternative fuels property data. This listing is intended to be illustrative rather than exhaustive; however, the literature incorporated herein provides a reasonably good cross-section of the available properties data base for petroleum-derived and synthetic liquid fuels and fuel gases.

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2. Navy Synthetic Fuels Reference File administered by Battelle Columbus Laboratories, Columbus, Ohio. Technical report and publication abstracting service, stored in mainframe computer and accesible via timesharing remote terminals.

3. Proceedings, 1981 International Gas Research Conference, Government Institutes, Inc., Rockville, MD., February 1982. Collection of papers on a variety of subjects relating to residential, commercial and industrial gas utilization. Includes descriptions of gas synthesization processes and products. First IGRC was held in 1979 and conferences are continuing on a biennial basis.

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APPENDIX C

FUELS PROPERTY DATA UPDATE QUESTIONNAIRE

As has been pointed out in Sections 4 and 5 of this report, an important first step in the development of an alternative fuels design data base is the collection of currently existing fuel properties and combustion performance data. This step serves to focus additional research on the apparent gaps in the data base while at the same time providing an initial base of design data in its own right. To carry out the consolidation of the available data, and the establish the objectives and schedules of ongoing programs designed to obtain fundamental fuel properties and combustion performance data, the questionnaires included in this appendix have been designed. These questionnaires are intended for circulation to individuals and laboratories known to be working in the appropriate areas, and request both specific data and references to original sources for additional data or more complete tabulations, etc. It should be kept in mind that these questionnaires are not intended to replace literature surveys as a source of design data base information, but to provide additional information and if possible, the results of ongoing work that has not yet been reported in the technical literature.

In the remainder of this appendix, a sample cover letter and questionnaire are provided to serve as a guide for a formal canvassing of research in this area.

(To responsible individual, laboratory
involved in fuels property or
combustion characteristics determination)

Subject: Alternative Fuels Design Data Base Assessment Project

Dear _____:

Under the sponsorship of the Jet Propulsion Laboratory, an alternative fuels design data base is currently being developed. As a necessary first step in this process, available data on alternative fuels properties and/or combustion characteristics is being solicited from research organizations such as yours known to be active in this area. The alternative fuels being considered include both synthetic liquids to replace petroleum-derived fuel oils and synthetic gases to replace natural gas. To accomplish this goal in the simplest possible manner, two questionnaires have been prepared, and are attached to this letter. The first of these requests specific fuels property data for alternative fuels, and also references to more complete data tabulations where they are available. The information requested is for a specific fuel; additional copies of the questionnaire may be used to provide data on other fuels that have been studied. Although specific units have been defined for each of the properties considered, any appropriate units may be used for the data requested.

The second questionnaire attached to this letter requests information of two types. First, for the specific combustion characteristics listed, the sources of alternative fuels data used in your work to obtain estimates of the individual characteristics prior to an experiment (i.e., in experiment or prototype burner design) are requested. Secondly, specific observations and literature citations with respect to the impact of alternative fuels on the combustion characteristics listed are also solicited.

Results of the circulation of these questionnaires and of an accompanying exhaustive literature search will be utilized to assemble a preliminary compilation of alternative fuels property data and of the impact of the use of alternative fuels on combustion characteristics important for industrial applications. Because of the importance of this objective to providing design information for industrial burner designers and thus to the long-term utilization of alternative fuels, your cooperation in returning these questionnaires is requested. All respondents will, of course, receive copies of the completed data base document.

Sincerely,

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QUESTIONNAIRE I

Alternative Fuel Properties Data

Please provide appropriate data, where avaiable, from your laboratory's work for the properties listed. Do not provide "handbook" data used in conjunction with measurements made in your laboratory in this questionnaire, but if such data are used, please note the source in the appropriate column. If data available are more extensive than space in this questionnaire allows, please append more detailed tabulations.

Fuel Type: __________

QI-1

Property	Property Value	Range	Source
I. COMPOSITION			
1. Elemental Composition			
C (wt %)			
H			
N			
S			
O			
Asn			
2. Hydrocarbon Types -			
ASTM D1319 & D2789			
Saturates			
• Straight Chain			
• Branched Chain			
• Cyclic Alkanes			

Property	Property Value	Range	Source
Olefins			
Aromatics- ASTM D1319			
3. Species			
4. Mean Molecular Formula			
5. Mean Molecular Weight- ASTM D2503			
II. PHYSICAL & THERMO-CHEMICAL PROPERTIES			
1. Density (g/cm^3) @ _____K (ASTM D287)			
2. Viscosity (Kinematic) (cm^3/s) @ _____ K @ _____ K (ASTM D240)			
3. Surface Tension (dynes/cm) @ _____ K			

Property	Property Value	Range	Source
4. Liquid Heat Capacity (cal/g°K) @ _____ K			
5. Heat of Combustion (lower heating value) (Kcal/g) ASTM D240			
6. Heat of Vaporization @ mean boiling point (cal/g)			
7. Distillation Data (°K) @ 1 atm ASTM D86 IBP 10% (Vol) 30% 50% 70% 90%			
8. Heat Capacity of Gas _____ K (cal/g°K)			
9. Viscosity of Gas _____ K (g/cm sec)			
10. Thermal Conductivity of Gas _____ K (cal/sec cm°K)			

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Property	Property Value	Range	Source
11. Diffusivity D_{fuel,N_2} (cm^2/sec)			
12. ΔS_F (cal/mol.K)			
III. STANDARD TEST/ PROCEDURE RESULTS			
1. Pour Point (°K) ASTM D97			
2. Flash Point (°K) ASTM D93			
3. Luminometer No. ASTM D1740			
4. Smoke Point ASTM D1322			
5. Water Content (% wt) ASTM D1796			
6. Sediment Content (% wt) ASTM D1796 & D473			
7. Metals Content (ppm wt)			
8. Asphaltenes (% wt)			
9. Ash (% wt) ASTM D482			
10. Existent Gum (mg/100 ml) ASTM 2274 & D381			

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QUESTIONNAIRE II

Alternative Fuel Combustion Characteristics

The information being sought with this questionnaire relates to two areas of great importance in the development of an alternative fuels design data base. These two areas are the sources of data currently in use to provide estimates of the combustion characteristic quantities of interest, and observations of the effects of alternative fuels on the listed characteristics. Clearly these two areas can be rather extensive, so that what is sought with this questionnaire is a summary of the information requested and a listing of appropriate technical references.

Fuel Type: __________

QII-1

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
I. Liquid Fuel Combustion			
1. Droplet and Spray Formation			
a) empirical correlations used			
b) observed accuracy of correlations			
c) observed effects of alternative fuels on spray formation			
d) specific studies of phenomenon			

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
2. Droplet Vaporization & Burning a) correlations used b) observed correlation accuracy c) observed effects of alternative fuels as spray combustion d) specific studies of phenomena			
II. BASIC COMBUSTION CHARACTERISTICS 1. Ignition and Flame Stabilization a) correlations used b) observed correlation accuracy c) observed effects of alternative fuel on ignition and flame stabilization d) observed ignition, flame stabilization limits			

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
e) specific studies			
2. Flame Temperature			
a) correlations used			
b) observed correlation accuracy			
c) flame temperatures observed with alternative fuels			
d) specific studies			
3. Laminar Flame Speed			
a) correlations used			
b) observed correlation accuracy			
c) flame speeds observed with alternative fuels			
d) specific studies			
III. CHEMICAL KINETICS			
1. Combustion Completion			
a) correlations used, accuracy			
b) observed effects of alternative fuel in direct substitution			

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
c) design modifications, if any, to accommodate alternative fuels use			
d) specific studies			
2. Soot Emissions			
a) correlations used/accuracy			
b) observed effects of alternative fuel use			
c) Design modification to accommodate alternative fuels, if any			
d) specific studies			
3. NO_x & SO_x Emissions			
a) correlations used/accuracy			
b) observed effects of alternative fuels use			
c) design modification to accommodate alternative fuels, if any			

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
d) specific studies			
IV. OPERATIONAL & DURABILITY			
1. Thermal & Oxidative Stability			
a) correlations used/accuracy			
b) observed characteristics of alternative fuel			
c) observed effects on combustion, if any			
d) specific studies			
2. Fouling & Corrosion			
a) correlations used/accuracy			
b) observed characteristics of alternative fuel			
c) observed effects on combustion, if any			
d) specific studies			

TABLE 11. Combustion Experiments for Alternative Fuels Effects Determination.

EXPERIMENT TYPE	EXPERIMENT OUTPUT	RATIONALE	FUEL PROPERTY DATA REQUIRED FOR INTERPRETATION	MODELS REQUIRED FOR INTERPRETATION/SCALING
1. PLUG FLOW REACTOR ● GAS PHASE FUEL OR PREVAPORIZED; PREMIXED.	Species and temperature as function of time, inlet temperature, fuel/air ratio, pressure, heat loss. Ignition delay time. Intermediate species, NO_x, SO_x, soot. Combustion completion time.	Kinetics data; ignition data. Determine key intermediates, relationship between intermediates and NO_x, SO_x, soot. CO/HC emissions data.	Fuel composition. Fuel thermodynamic properties.	One-dimensional plug flow analysis. Finite-rate chemical kinetics formulation.
2. WELL-STIRRED REACTOR (a) GAS PHASE FUEL OR PREVAPORIZED, PREMIXED.	Species as function of residence time, inlet temperature, fuel/air ratio, pressure, heat loss. Emissions characteristics-NO_x, SO_x, soot. Blowout limits.	Kinetics data, emissions characterization, soot limits, combustion stability limits.	Fuel composition. Fuel thermodynamic properties.	Well-stirred reactor analysis. Finite-rate chemical kinetics formulation.
(b) LIQUID PHASE FUEL	As above, as function of spray quality.	Effect of liquid fuel properties on emissions, sooting, combustion stability.	As above, with liquid fuel properties, spray characteristics.	Multiphase well-stirred reactor analysis. Finite-rate chemical kinetics formulation. Droplet vaporization/burning model. Residence-time distribution function model.
3. LAMINAR & TURBULENT FLAMES ● GAS PHASE FUEL OR PREMIXED. (a) FLAT FLAME, PREMIXED.	Flame speed, species and temperature histories. Intermediate species, NO_x, SO_x, soot, as function of inlet fuel/air ratio, temperature, heat loss.	Reactivity determination, relative to fuel type, fuel/air ratio, temperature. Data for kinetics model development. Interaction of chemical kinetics with laminar and turbulent flowfield, transport properties. Effects of transport property variation. Ignition/stabilization limits.	Fuel composition. Fuel thermodynamic properties. Gas-phase transport properties. Effective emissivities for gas phase, soot.	Laminar flat flame model, with effects of diffusion, chemical kinetics, variable transport properties. Radiation heat loss model.
(b) DIFFUSION FLAME ● PARTIALLY PREMIXED AND PURE DIFFUSION.	As above.	As above.		Laminar bunsen flame model, parabolic steady-state and elliptic time-dependent, with effects of diffusion, chemical kinetics, radiation heat loss.
4. SINGLE DROPLET COMBUSTION (a) OPTICAL MEASUREMENTS.	Drop diameter as a function of time, ambient temperature, fuel type.	Burning rate coefficient and transfer number determination.	Fuel type.	Classical single drop model.
(b) DETAILED MEASUREMENTS.	As above, with detailed measure of species evolved in vaporization, burning of drop. Pyrolysis of droplet. Formation of cenospheres. Drop temperature as function of time.	As above. Investigate fuel pyrolysis, formation of cenospheres as function of fuel type, ambient environment. Data for detailed drop combustion model. Kinetics of fuel decomposition.	Fuel composition, thermodynamic properties, liquid-phase physical properties.	Detailed nonuniform temperature multicomponent fuel droplet combustion model. Finite-rate kinetics formulation.

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TABLE 11. Combustion Experiments for Alternative Fuels Effects Determination (continued).

EXPERIMENT TYPE	EXPERIMENT OUTPUT	RATIONALE	FUEL PROPERTY DATA REQUIRED FOR INTERPRETATION	MODELS REQUIRED FOR INTERPRETATION/SCALING
5. COMBINED WSR/PLUG FLOW WITH DISTRIBUTED INJECTION (a) GAS PHASE FUEL OR PREVAPORIZED.	Exit species as function of residence time, inlet temperature, fuel/air ratio, primary/secondary air injection rate, heat exchange in plug flow.	Examine in controlled simulation effects of aerodynamics and staging in combustion process as a function of fuel type. Determine techniques for minimizing NO_x, SO_x, soot. Investigate quenching effects.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data.	Coupled well-stirred reactor/plug flow with distributed injection in plug flow. Finite-rate chemical kinetics.
(b) LIQUID PHASE FUEL	As above, as function of fuel liquid properties, fuel type.	As above. Examine effects of air preheat on combustion process for liquid fuels.	As above, with liquid fuel properties, spray characterization.	Multiphase well-stirred reactor/plug flow with distributed injection model. Finite-rate chemical kinetics, droplet combustion model.
6. SPRAY CHARACTERIZATION	Droplet size, distribution as function of injector type, fuel type, fuel temperature, pressure, primary and secondary air flow rate.	Determine influence of fuel properties on spray droplet size and droplet distribution function. Investigate interaction of spray injector, fuel type, and airflow velocity as affects drop size.	Fuel liquid-phase physical properties.	Spray formation analysis - numerical or semiempirical.
7. SPRAY VAPORIZATION/ BURNING - UNIFORM FLOW	Combustion characteristics - species profiles, SO_x, NO_x, soot; temperature as function of fuel spray quality, air temperature, heat transfer rates; simplified aerodynamics.	Determine overall effects of fuel properties on combustion processes in simplified model burner simulation. Investigate effects of air preheat, staging, for spray fuel injection.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data. Effective thermal emissivity. Fuel liquid properties. Spray characterization.	Spray transport/vaporization/burning analytical model. Coupled finite-rate chemistry; single droplet and spray burning models.
8. ALTERNATIVE FUELS COMBUSTION IN A MODEL BURNER (a) GAS PHASE FUEL OR PREVAPORIZED.	Combustion characteristics - species profiles, NO_x, SO_x, soot, temperature as function of fuel type, fuel/air ratio, air temperature, heat transfer rates, representative burner aerodynamics: large scale recirculation zones, swirl.	Determine overall effects of alternative fuels on combustion processes in aerodynamics representative of industrial burners.	Fuel composition. Fuel thermodynamic properties. Chemical kinetic rate data. Effective thermal emissivity.	Industrial burner combustion model: turbulent mixing, recirculation zones, swirl, coupled finite-rate chemistry.
(b) LIQUID PHASE FUEL	As above, with addition of spray quality as a parameter.	As above, with addition of spray injection representative of industrial liquid-fuel burners.	As above, with addition of: Fuel liquid properties. Spray characterization.	Multiphase industrial burner combustion model; add spray transport to above specification.

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TABLE 12

SUGGESTED DATA BASE DEVELOPMENT PLAN BY PHASE AND TASK

PHASE	TASKS	OUTPUT
Basic Data Generation	Thermodynamic properties compilation Fuel composition data compilation Chemical kinetic rate determination Single droplet combustion Fuel liquid properties compilation Spray characterization	Basic composition, physical and thermodynamic property data compilation Droplet burning rate data Drop size/distribution data
Preliminary Properties Effects Determination	Multiphase well-stirred reactor experiments Single droplet combustion (detailed data) Well-stirred reactor/plug flow experiments (gas phase and multiphase)	Effects of fuel properties on the combustion process simplified systems
Alternative Fuel Effects in Industrial Burners	Well-stirred reactor/plug flow experiments (gas phase, multiphase) Spray vaporization and burning in uniform flow Model industrial burner experiments	Effects of fuel properties on the combustion process in realistic systems.

compilation of fuel composition data, for with appropriate composition data it is possible to estimate fuel properties where measured properties are not available. These estimated fuel properties can then be used in the analysis of the combustion experiments listed in Table 11, and the results of this analysis will, in turn, indicate the sensitivity of the particular combustion process to the estimated property value. This iterative procedure will allow the definition of those fuel properties for which estimated values are insufficiently accurate. More accurate values obtained by experimental measurement could then be obtained and used for further data analysis.

The basic data generation phase of the suggested program includes the stirred reactor and plug flow combustion experiments, single droplet combustion experiments, spray characterization experiments, and liquid properties data compilation work in addition to the composition, thermodynamic, and physical properties data compilations already discussed. These basic experiments would provide the data, including chemical kinetic and liquid burning rate information, and spray droplet size and distribution, necessary to provide at least a preliminary assessment of the effects of alternative fuels on combustion processes relevant to industrial burner design.

To obtain more refined estimates of alternative fuels effects on the combustion processes relevant to industrial burner design, the work outlined under the preliminary properties effects determination phase would be carried out. Because a primary impact of alternate fuels with respect to industrial burners is anticipated to involve liquid fuel combustion processes, this phase incorporates multiphase well-stirred reactor experiments (which require the spray characterization work carried out in the preceding phase for their analysis and interpretation) and more detailed single droplet experiments. For both gas phase alternative fuels and liquid fuels, the well-stirred reactor-plug flow experiments would provide an initial data base on the effects of aerodynamics, staging, inlet air heating, and other emissions control efficiency improvement techniques on the combustion process. Thus, the overall output of this phase would be an initial evaluation of the effects of fuel properties on the combustion process in simplified systems that incorporate some of the important features of industrial burners. Note that the properties data base, kinetics data base, and liquid fuel combustion processes data base obtained in the initial phase of the suggested program are all necessary for the evaluation of the data obtained during this phase.

The the third phase of the suggested program would be designed to provide a comprehensive quantification of the effects of the use of alternative fuels in industrial burners. This phase, as shown in Table 12, incorporates additional well-stirred reactor/plug flow reactor experiments, experimental investigations of spray combustion in a uniform flow, and experiments in a configuration designed to model the flowfield in a representative industrial burner. The output of this phase is then a description of the effects of fuel properties on the combustion process in realistic systems. Taken together, the suggested program will thus provide a complete and comprehensive evaluation of the impact of the use of alternative fuels on industrial burner design.

Each of the experimental efforts outlined in Table 11 interacts to some extent with the other tasks of the suggested work, as is noted in the column entitled "Fuel property data required for interpretation" in Table 11. Because of these interactions, certain of the tasks must follow the availability of data from other tasks, as is depicted in the phase/task/time interaction diagram, Fig. 25. As is shown in this figure, the initial tasks involve thermodynamic and physical properties compilation and composition data compilation, as well as single-droplet burning rate determination. This is not meant to imply that no other work can be initiated until the properties data compilation is completed, since as outlined above, certain physical and chemical properties of the fuel may be adequately estimated. Further, for many alternative fuels of interest an initial data base encompassing thermodynamic and physical properties, as well as single-droplet burning rate data already exists. Thus, although not shown in Fig. 25 explicitly, a concurrent assessment of available data should be carried out with this phase of the suggested program.

As the interactions shown on Fig. 25 suggest, there is a considerable degree of relationship between each of the tasks shown. This figure does not indicate a feedback of information between tasks, but such a feedback is a basic requirement for any well-constructed program and would be anticipated in any program structured along the lines suggested in this report.

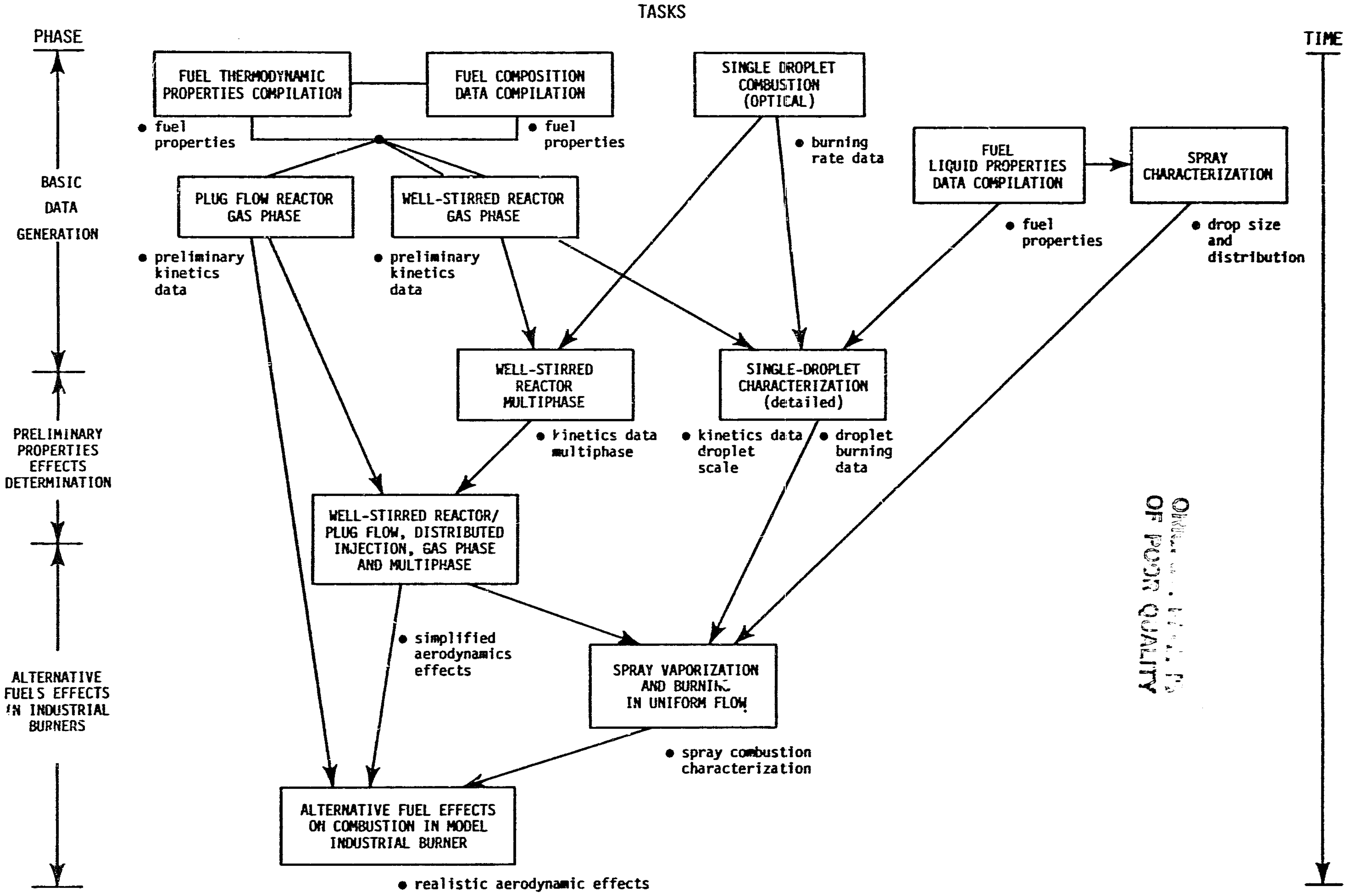

FIGURE 25. Phase-Task-Time Interaction Diagram - Alternative Fuels Effects Determination.

6. NEW TECHNOLOGY

No reportable items of new technology have been developed as part of the work reported in this document.

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APPENDIX A

FUEL PROPERTY DATA AND DATA FORMAT

As noted in the text of this report, accurate fuel composition, thermodynamic, and physical properties data is required for alternate fuels in order to assess the impact of the utilization of these fuels on industrial burner design. Assessment of the composition and properties of SRC-II mid-distillate and heavy distillate, and No. 2 and No. 6 fuel oil, is a portion of the effort being carried out in a current Department of Energy sponsored program at SAI [A1]. This work has involved both compilation of available experimental property data and estimation of these quantities where experimental data were not available. The estimation techniques used are described in Ref. A1. Some of the results of this current work are presented in this appendix as an example of data needs and data format for reporting this information.

A comprehensive summary of the property data for SRC-II MD, SRC-II HD, No. 2 fuel oil and No. 6 fuel oil is presented in Table A1. Where data have been estimated, the symbol (E) is used. It should be noted that the estimates shown in Table A1 are based on preliminary composition data and can be refined as more specific composition data becomes available. The data in this table show that SRC-II MD and No. 2 fuel oil have similar properties except for the C/H ratio and the oxygen and nitrogen content: these differences can be expected to affect the chemical kinetic behavior primarily, and could lead to greater soot and NO_x emissions from SRC-II MD than from No. 2 fuel oil.

Measured data are available for all properties except the surface tension and liquid heat capacity of No. 6 fuel oil, the heat of vaporization for all the fuels considered, the gas phase properties of each fuel, and the standard entropy of formation of these fuels. Reasonable estimates of these properties can be made using the techniques described in Ref. A1, but experimental verification of the estimated values should be carried out, especially with respect to the gas phase transport properties.

Although the data shown in Table A1 are available or can be estimated, no information is incorporated on temperature variation of the physical properties listed. This is a major difficulty: while the data available do allow

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TABLE A1. Fuel Property Data and Data Format.

	SRC-II MD	SRC-II HD	NO. 2 FUEL OIL	NO. 6 FUEL OIL
ELEMENTAL COMPOSITION				
C (WT %)	84.59	88.98	86.4	87.2
H	8.84	7.64	13.3	11.96
N	0.85	1.03	0	0.46
S	0.20	0.39	0.3	0.47
O	5.43	1.9	0	0.86
ASH	0.002	0.058	0.001	0.008
HYDROCARBON TYPES-ASTM D1319 & D2789				
SATURATES				
• STRAIGHT CHAIN	0		70.5	
• BRANCHED CHAIN	0		7.5	
• CYCLIC ALKANES	35			
OLEFINS	0		0	
AROMATICS-ASTM D 319	65		22	
SPECIES:	CRESOL XYLENOL METHYLNAPHTHALENE DIMETHYLNAPHTHALENE NAPHTHALENE TRIMETHYLPHENOL TETRALIN PHENOL METHYLTETRALIN OTHERS	ANTHRACENE PYRENE METHYLANTHRACENE METHYLPYRENE DIMETHYLBIPHENYL TRIMETHYLBIPHENYL METHYLBIPHENYL FLUORINE DIMETHYLPYRENE OTHERS	C_{12}-C_{17} N-PARAFFINS TRIMETHYLDODECANE METHYLINDAN TETRALIN METHYLTETRALIN METHYLACENAPHTHENE TETRAETHYLBENZENE METHYLPROPYLBENZENE METHYLNAPHTHALENE DIMETHYLNAPHTHALENE OTHERS	C_{18}-C_{43} N-PARAFFINS CYCLIC ALKANES AND POLYAROMATICS C_{18}-C_{53}
MEAN MOLECULAR FORMULA	$C_{12}H_{15}O_{0.6}N_{0.1}S_{0.01}$	$C_{14}H_{12.4}O_{0.2}N_{0.1}S_{0.02}$	$C_{13}H_{22}S_{0.02}$	$C_{22.8}H_{37.6}N_{0.10}S_{0.05}O_{0.17}$
MEAN MOLECULAR WEIGHT-ASTM D2503	169	185	178	315
DENSITY (g/cm³)-ASTM D287				
@ 288°K	0.974	1.09	0.844	0.915
KINEMATIC VISCOSITY (cm³/s)-ASTM D445				
@ 333.3°K	0.0306	0.121	0.0350	0.29
@ 371.9°K	0.0134	0.0473	0.0149	
SURFACE TENSION (dynes/cm)				
@ 295°K	33	28.5	29.9	35.3 (E)†
LIQUID HEAT CAPACITY (cal/g °K)				
@ 394°K	0.55	0.41	0.53	0.53 (E)†
HEAT OF COMBUSTION (LOWER HEATING VALUE) (Kcal/g) ASTM D240	8.994	9.122	10.161	9.88

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TABLE A1. Fuel Property Data and Data Format (continued).

	SRC-II MD	SRC-II HD	NO. 2 FUEL OIL	NO. 6 FUEL OIL
HEAT OF VAPORIZATION @ MEAN BOILING POINT (cal/g) (E)	64.2 (E)	70.3 (E)	61.5 (E)	48.3 (E)†
DISTILLATION DATA @ 1 atm (°K)				
IBP - ASTM D86	473	563	472	506
10% (Vol)	481	580	490	589
30%	492	598	515	644
50%	502	620	533	700
70%	512	652	554	756
90%	533	700	584	867
HEAT CAPACITY OF GAS 650°K (cal/g °K) (E)	0.564	0.465	0.663	0.64†
VISCOSITY OF GAS 650°K (g/cm sec) (E)	1.17×10^{-4}	1.22×10^{-4}	1.15×10^{-4}	$1.27 \times 10^{-4\dagger}$
THERMAL CONDUCTIVITY OF GAS 650°K (cal/sec cm °K)	6.38×10^{-5} (E)	6.84×10^{-5} (E)	8.81×10^{-5} (E)	$9.32 \times 10^{-5\dagger}$ (E)
DIFFUSIVITY (cm^2/sec) (E) $D_{fuel,\ N_2}$	2.03×10^{-1}	1.60×10^{-1}	2.02×10^{-1}	$1.75 \times 10^{-1\dagger}$
ΔS_F (cal/mol · K) (E)	120.84	107.34	140.15	$\dagger$
TEST PROCEDURE				
POUR POINT (°K) ASTM D97	230.2	280.2	252.4	300
FLASH POINT (°K) ASTM D93	358	441	345	473
LUMINOMETER NO. ASTM D1740	2.0	-	29.0	
SMOKE POINT ASTM D1322	8.0	-	16.0	
WATER CONTENT (% WT) ASTM D1796	0.1 - 0.6	1.48	0	0.07
SEDIMENT CONTENT (% WT) ASTM D1796 & D473	0 - 0.05	0.02	0	0.052
METALS CONTENT (PPM WT)	(FOR A BLEND OF MD & HD)			
	TITANIUM 0.5	VANADIUM 0.23	0	
	SODIUM 1.4	LEAD 0.12		
ASPHALTENES (% WT)	POTASSIUM 1.5	IRON 13	0	1.3 - 8.0
	CALCIUM 1.6	PHOSPHORUS < 0.01		
ASH (% WT)- ASTM D482	0.002	0.028	< 0.001	0.02
EXISTENT GUM (mg/100 ml)-ASTM 2274 & D381	0.8	0	0.9, 10.7	

†ESTIMATED VALUES FOR NO. 6 FUEL OIL WERE MADE WITH THE CHARACTERIZATION FACTOR METHOD. CORRELATIONS FOR ΔS_F ARE NOT AVAILABLE USING THIS METHOD.

(E) = ESTIMATED VALUES.

first-order estimates of some of the effects of alternative fuels such as listed in Table A1 on industrial burner design to be made, more reliable estimates, as noted in Section 2 of this report, require the temperature variation information. Thus, the data shown in Table A1, while it establishes a useful baseline, does not provide the complete suite of data required to fully assess alternative fuels effects on burner design.

APPENDIX B

ANNOTATED BIBLIOGRAPHY

The reports, papers, books, and conference or symposium proceedings listed in this appendix provide a variety of sources of alternative fuels property data. This listing is intended to be illustrative rather than exhaustive; however, the literature incorporated herein provides a reasonably good cross-section of the available properties data base for petroleum-derived and synthetic liquid fuels and fuel gases.

1. Fossil Energy Update, U.S. Dept. of Energy, Technical Information Center, Oak Ridge, Tennessee. Monthly. Available via subscription as PB82-914600 from the National Technical Information Service, Springfield, VA. 22161. Abstracting and index periodical. Subject matter includes coal, petroleum, natural gas, oil shale, hydrogen production, hydrocarbon and alcohol fuels, electric power engineering, magnetohydrodynamic generators, fuel cells, combustion systems and combustion chemistry.

2. Navy Synthetic Fuels Reference File administered by Battelle Columbus Laboratories, Columbus, Ohio. Technical report and publication abstracting service, stored in mainframe computer and accesible via timesharing remote terminals.

3. Proceedings, 1981 International Gas Research Conference, Government Institutes, Inc., Rockville, MD., February 1982. Collection of papers on a variety of subjects relating to residential, commercial and industrial gas utilization. Includes descriptions of gas synthesization processes and products. First IGRC was held in 1979 and conferences are continuing on a biennial basis.

4. Selected Values of Properties of Hydrocarbons and Related Compounds, Texas A&M University, College Station, TX. 1981. The current edition of American Petroleum Institute Project 44. Only the recent work on this project includes properties (of pure species) at high enough temperatures to be useful for combustion applications.

5. Solvent Refined Coal (SRC) Process, Pittsburgh and Midway Coal Corp., DOE/FE-496-109 through -496-176, October 1975-February 1980, and DOE/ET/10104-8, Sept. 1980. Detailed data on SRC-II fuel characteristics.

6. Standard Specification for Fuel Oils, ASTM D396-80 (1980). Provides all current ASTM standards for fuel oils.

7. Symposium Papers: New Fuels and Advances in Combustion Technologies, Institute of Gas Technology, Chicago, IL., June 1979. Proceedings of a technical symposium with primary emphasis on synthetic gases, gas from biomass, etc., and the systems and combustion problems encountered with their utilization.

8. *Symposium Papers: Advances in Coal Utilization Technology, Institute of Gas Technology, Chicago, IL., June 1979.* Symposium proceedings focusing on coal utilization. Some papers on production of synthetic fuels from coal.

9. *Symposium Papers: Synthetic Fuels from Oil Shale, Institute of Gas Technology, Chicago, IL., December 1980.* Proceedings of technical symposium focusing on both liquid and gaseous synthetic fuels. Includes both production techniques and products, and examinations of combustion characteristics and effects of the use of the fuels.

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14. Bowden, J.N. and D.W. Brinkman, "Stability Survey of Hydrocarbon Fuels," DOE/BETC/1778-4, Oct. 1979. Stability data for No. 2 diesel, JP-4 and gasoline are presented.

15. Bowden, J.N. and D.W. Brinkman, "Stability Characteristics of Some Shale and Coal Liquids," DOE/BETC/4162-10, Nov. 1980. Data on shale oil and EDS.

16. Brinkman, D.W., M.L. Whisman and J.N. Bowden, "Stability Characteristics of Hydrocarbon Fuels from Alternative Sources," DOE/BETC/RI-78/-23, March 1979. Stability characteristics of gasoline and jet fuel derived from coal, tar sands and oil shale are presented.

17. Brinkman, D.W., J.N. Bowden and H.N. Giles, "Crude Oil and Finished Fuel Storage Stability: An Annotated Review," DOE/BETC/RI-79/13, Feb. 1980. Petroleum fuels only.

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APPENDIX C

FUELS PROPERTY DATA UPDATE QUESTIONNAIRE

As has been pointed out in Sections 4 and 5 of this report, an important first step in the development of an alternative fuels design data base is the collection of currently existing fuel properties and combustion performance data. This step serves to focus additional research on the apparent gaps in the data base while at the same time providing an initial base of design data in its own right. To carry out the consolidation of the available data, and the establish the objectives and schedules of ongoing programs designed to obtain fundamental fuel properties and combustion performance data, the questionnaires included in this appendix have been designed. These questionnaires are intended for circulation to individuals and laboratories known to be working in the appropriate areas, and request both specific data and references to original sources for additional data or more complete tabulations, etc. It should be kept in mind that these questionnaires are not intended to replace literature surveys as a source of design data base information, but to provide additional information and if possible, the results of ongoing work that has not yet been reported in the technical literature.

In the remainder of this appendix, a sample cover letter and questionnaire are provided to serve as a guide for a formal canvassing of research in this area.

(To responsible individual, laboratory
involved in fuels property or
combustion characteristics determination)

Subject: Alternative Fuels Design Data Base Assessment Project

Dear _____:

Under the sponsorship of the Jet Propulsion Laboratory, an alternative fuels design data base is currently being developed. As a necessary first step in this process, available data on alternative fuels properties and/or combustion characteristics is being solicited from research organizations such as yours known to be active in this area. The alternative fuels being considered include both synthetic liquids to replace petroleum-derived fuel oils and synthetic gases to replace natural gas. To accomplish this goal in the simplest possible manner, two questionnaires have been prepared, and are attached to this letter. The first of these requests specific fuels property data for alternative fuels, and also references to more complete data tabulations where they are available. The information requested is for a specific fuel; additional copies of the questionnaire may be used to provide data on other fuels that have been studied. Although specific units have been defined for each of the properties considered, any appropriate units may be used for the data requested.

The second questionnaire attached to this letter requests information of two types. First, for the specific combustion characteristics listed, the sources of alternative fuels data used in your work to obtain estimates of the individual characteristics prior to an experiment (i.e., in experiment or prototype burner design) are requested. Secondly, specific observations and literature citations with respect to the impact of alternative fuels on the combustion characteristics listed are also solicited.

Results of the circulation of these questionnaires and of an accompanying exhaustive literature search will be utilized to assemble a preliminary compilation of alternative fuels property data and of the impact of the use of alternative fuels on combustion characteristics important for industrial applications. Because of the importance of this objective to providing design information for industrial burner designers and thus to the long-term utilization of alternative fuels, your cooperation in returning these questionnaires is requested. All respondents will, of course, receive copies of the completed data base document.

Sincerely,

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QUESTIONNAIRE I

Alternative Fuel Properties Data

Please provide appropriate data, where avaiable, from your laboratory's work for the properties listed. Do not provide "handbook" data used in conjunction with measurements made in your laboratory in this questionnaire, but if such data are used, please note the source in the appropriate column. If data available are more extensive than space in this questionnaire allows, please append more detailed tabulations.

Fuel Type: ________

QI-1

Property	Property Value	Range	Source
I. COMPOSITION			
1. Elemental Composition			
C (wt %)			
H			
N			
S			
O			
Asn			
2. Hydrocarbon Types -			
ASTM D1319 & D2789			
Saturates			
● Straight Chain			
● Branched Chain			
● Cyclic Alkanes			

Property	Property Value	Range	Source
Olefins			
Aromatics- ASTM D1319			
3. Species			
4. Mean Molecular Formula			
5. Mean Molecular Weight- ASTM D2503			
II. PHYSICAL & THERMO-CHEMICAL PROPERTIES			
1. Density (g/cm^3) @ _____ K (ASTM D287)			
2. Viscosity (Kinematic) (cm^3/s) @ _____ K @ _____ K (ASTM D240)			
3. Surface Tension (dynes/cm) @ _____ K			

Property	Property Value	Range	Source
4. Liquid Heat Capacity (cal/g°K) @ _____ K			
5. Heat of Combustion (lower heating value) (Kcal/g) ASTM D240			
6. Heat of Vaporization @ mean boiling point (cal/g)			
7. Distillation Data (°K) @ 1 atm ASTM D86			
IBP			
10% (Vol)			
30%			
50%			
70%			
90%			
8. Heat Capacity of Gas _____ K (cal/g°K)			
9. Viscosity of Gas _____ K (g/cm sec)			
10. Thermal Conductivity of Gas _____ K (cal/sec cm°K)			

Property	Property Value	Range	Source
11. Diffusivity D_{fuel,N_2} (cm^2/sec)			
12. ΔS_F (cal/mol.K)			
III. STANDARD TEST/ PROCEDURE RESULTS			
1. Pour Point (^{o}K) ASTM D97			
2. Flash Point (^{o}K) ASTM D93			
3. Luminometer No. ASTM D1740			
4. Smoke Point ASTM D1322			
5. Water Content (% wt) ASTM D1796			
6. Sediment Content (% wt) ASTM D1796 & D473			
7. Metals Content (ppm wt)			
8. Asphaltenes (% wt)			
9. Ash (% wt) ASTM D482			
10. Existent Gum (mg/100 ml) ASTM 2274 & D381			

QUESTIONNAIRE II

Alternative Fuel Combustion Characteristics

The information being sought with this questionnaire relates to two areas of great importance in the development of an alternative fuels design data base. These two areas are the sources of data currently in use to provide estimates of the combustion characteristic quantities of interest, and observations of the effects of alternative fuels on the listed characteristics. Clearly these two areas can be rather extensive, so that what is sought with this questionnaire is a summary of the information requested and a listing of appropriate technical references.

Fuel Type: __________

QII-1

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
I. Liquid Fuel Combustion			
1. Droplet and Spray Formation			
a) empirical correlations used			
b) observed accuracy of correlations			
c) observed effects of alternative fuels on spray formation			
d) specific studies of phenomenon			

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
2. Droplet Vaporization & Burning a) correlations used b) observed correlation accuracy c) observed effects of alternative fuels as spray combustion d) specific studies of phenomena			
II. BASIC COMBUSTION CHARACTERISTICS 1. Ignition and Flame Stabilization a) correlations used b) observed correlation accuracy c) observed effects of alternative fuel on ignition and flame stabilization d) observed ignition, flame stabilization limits			

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
e) specific studies			
2. Flame Temperature			
a) correlations used			
b) observed correlation accuracy			
c) flame temperatures observed with alternative fuels			
d) specific studies			
3. Laminar Flame Speed			
a) correlations used			
b) observed correlation accuracy			
c) flame speeds observed with alternative fuels			
d) specific studies			
III. CHEMICAL KINETICS			
1. Combustion Completion			
a) correlations used, accuracy			
b) observed effects of alternative fuel in direct substitution			

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Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
c) design modifications, if any, to accommodate alternative fuels use			
d) specific studies			
2. Soot Emissions			
a) correlations used/accuracy			
b) observed effects of alternative fuel use			
c) Design modification to accommodate alternative fuels, if any			
d) specific studies			
3. NO_x & SO_x Emissions			
a) correlations used/accuracy			
b) observed effects of alternative fuels use			
c) design modification to accommodate alternative fuels, if any			

Combustion Characteristic	Design/Development Estimation Procedure	Observations	References
d) specific studies			
IV. OPERATIONAL & DURABILITY			
1. Thermal & Oxidative Stability			
a) correlations used/accuracy			
b) observed characteristics of alternative fuel			
c) observed effects on combustion, if any			
d) specific studies			
2. Fouling & Corrosion			
a) correlations used/accuracy			
b) observed characteristics of alternative fuel			
c) observed effects on combustion, if any			
d) specific studies			