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Combustion and Environmental Challenges for Gas Turbines in the 1990s

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I. Introduction

THE close resemblance between various gas turbine combustors, evolved over the last 50 yr, have been dictated largely by the length and frontal area to remain within the limits set by other engine components, and incorporation of a diffuser (to minimize pressure loss) and liner (to provide stable operation over a wide range of air/fuel ratios). Despite the continued advances in gas turbine combustor technology, the challenge which a combustion engineer faces today to ingenuity in design is greater than ever before. Interest in the environment has evolved from the gradual deterioration in our air quality and the discovery of the antarctic ozone hole, in addition to hot summers, the greenhouse effect, and increased smog in the cities. In addition, energy conservation and higher efficiency remains on the priority list.

New advanced concepts and technology are still needed to satisfy the current and projected pollutants emission regulations and to operate combustors with a broader range of fuels. These fuels are generally of poorer grade with higher C/H ratio and aromatic content. This change has not provided any relaxation to the more conventional requirements of durability, pattern factor, stability, relighting capability, high combustion efficiency, etc. In fact, except for relighting, these requirements have become more stringent as operating temperatures within the hot section of the engine have continued to rise, and are expected to continue to rise in the near future.[1,2] The combustion efficiencies demanded by current pollutant legislation imply combustor loadings at the engine idling condition that are often more severe than relighting requirements, so that the sizing of the combustor may now be dictated by pollution constraints.

In addition to the above externally imposed demands, combustor improvements are required that keep pace with the development of other key engine components. Reduction of combustor length, size, and weight is expected to continue to be an important requirement. The desired performance requirements, in terms of higher engine thrust/weight ratio and lower specific fuel consumption, will call for higher turbine inlet temperatures and closer fit to the design temperature profile at inlet to the turbine. In addition, it is expected that

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the demand for greater reliability, increased durability, and lower manufacturing, development, and maintenance costs, fuel economy, fuel flexibility, and lower levels of pollutants emission will assume added importance in the future. In order to meet these challenges, combustion engineers are expected to address basic issues and methods for advanced combustors. Major issues in the near term are expected to be with the environmental pollution, fuel flexibility, and fuel economy. The development will require detailed understanding of the fundamental processes, establishment of data bases, and advanced cooling methods.

The challenge of the sixties to the combustion engineer was increased power output, combustor durability, and performance for the larger size of propulsion systems. The environmental concern and the establishment of the U.S. Environment Protection Agency provided combustion engineers the challenge in the seventies of reducing or alleviating pollutants that adversely affect our environment. Major emphasis was placed on the gaseous pollutants. The challenge during the eighties was clearly energy conservation, combustor durability, and the associated design and development process using conventional and broad-based fuels. The challenges we expect to face in the nineties are environmental pollution reduction and energy conservation. Increased use is expected to be made of low-grade fuels and alternative fuels. Advanced combustion diagnostics, using state-of-the-art experimental and computational tools, is expected to provide significant advances in combustor design and development. The combustor length will become even shorter than it is at present so that concerns over energy release rate, pattern factor, and energy conservation will grow even more. Greater use of modeling and simulation techniques will be made for combustor development.

II. Environmental Pollution Problem

Environmental pollution occurs largely from transportation and industrial sources. Emissions of the so-called greenhouse gases, such as carbon dioxide and methane (and chloroflurocarbons), have sparked numerous debates on the potential for global warming, which could occur as a result of these gases accumulating in the atmosphere. The presence of oxides of hydrogen (HO_x) in the upper atmosphere as well as other engine exhaust gases (considered as pollutants) can destroy ozone. Atmospheric ozone forms a blanket around the Earth at a height of 10–30 miles and has the ability to absorb ultraviolet (uv) light from the Sun. Without the ozone layer, life on Earth would be dramatically different, because unblocked uv rays can kill plant and animal cells. Exhaust gas species contain not only CO_2, H_2O, hydrocarbons, and soot particles, but also several nitrogenous compounds, including NO_x (commonly grouped as NO, NO_2, N_2O), NO_3, N_2O_5, and HNO_3, oxides of sulfur (SO_x) and other and sulfur compounds. The total unburned hydrocarbons (THC) and CO in the exhaust plume represent not only combustion inefficiency, but also play an important role in stratospheric HO_x (OH and HO_2) chemistry (Fig. 1). Nitrous oxide (N_2O) and nitrogen dioxide (NO_2) diffusing upward from engine exhaust breaks into destructive nitric oxide (NO) in the atmosphere and accounts for about 50% of the ozone depletion. Stationary gas turbine powerplants also contribute to the problem of ozone depletion and acid rain (Fig. 1).

III. Oxides of Nitrogen Formation in Combustors

Most of the present day fuels used in gas turbine combustors have a negligible amount of fuel-bound nitrogen and sulfur so that only thermal NO_x and chemical sulfur oxides transformation are important. However, future synthetic or derived fuels can have small-to-moderate amounts of bound nitrogen. Temperature has a slight effect on fuel nitrogen conversion. The thermal NO_x contribution is small below temperatures of 1200°C, increasing at temperatures of 1400°C+. Peak flame temperature is often used as a guide to thermal NO_x production and can be controlled by the fuel and air mixing process, combustion intensity, residence time, local excess air level, local temperature, and combustion air preheat. The thermal NO_x has been shown to be exponentially dependent on temperature and linearly dependent upon time.

Not all the nitrogen in the fuel reacts to form NO_x. The evolution of the nitrogenous species from the fuel under reducing atmospheres favors the formation of N_2 rather than NO_x (Fig. 2). Pyrolysis compounds found in oxygen deficient areas of the flame can reduce NO_x back to N_2 (Figs. 3 and 4), as can reactions with later stages of flame with CO and carbon. Controlled fuel and air mixing is therefore the prin-

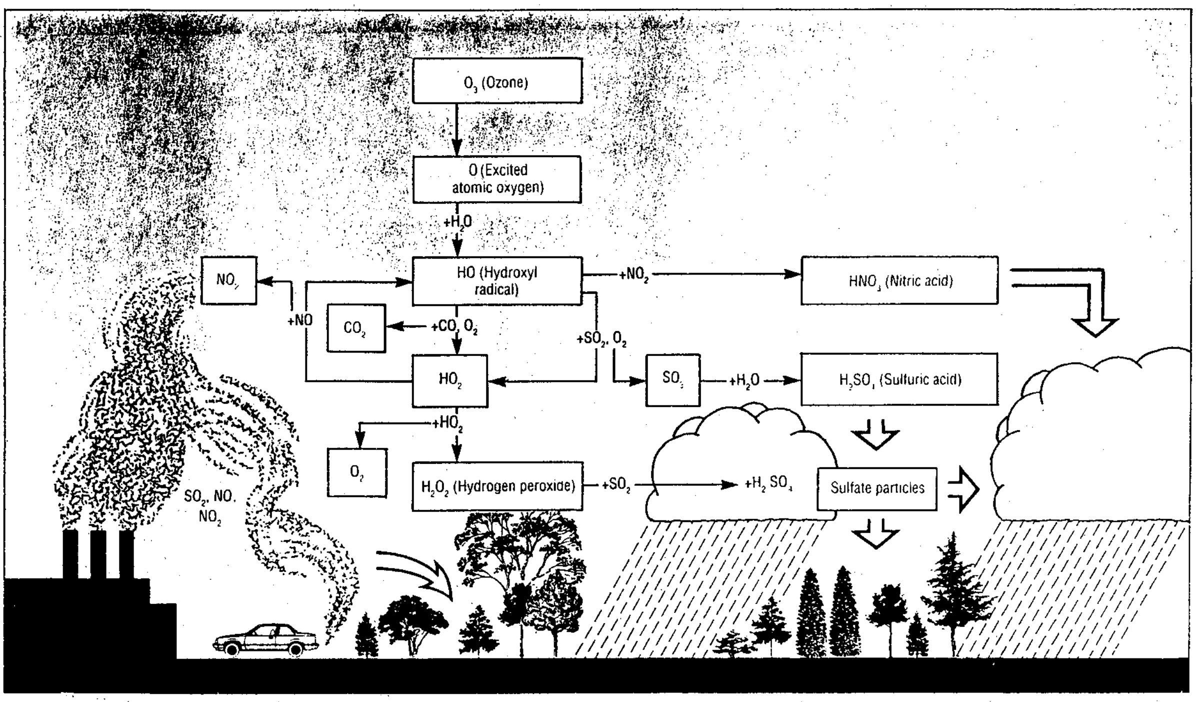


Fig. 1 Schematic diagram of ozone depletion and acid deposition.

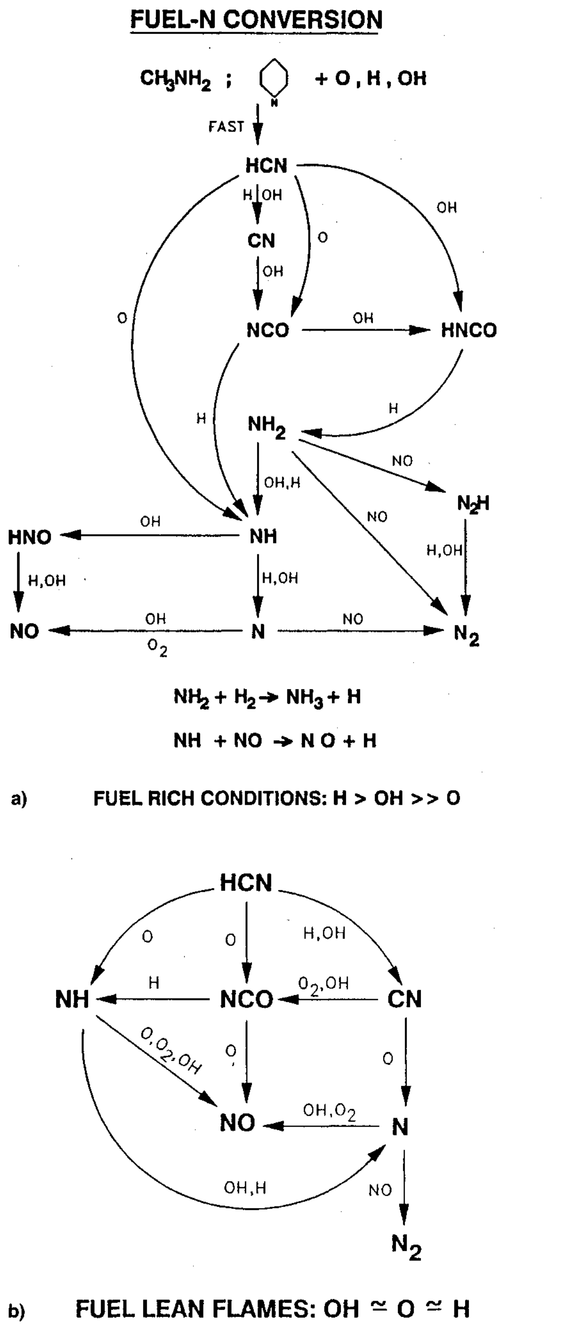


Fig. 2 Fuel nitrogen conversion: a) fuel rich conditions and b) fuel lean flames.

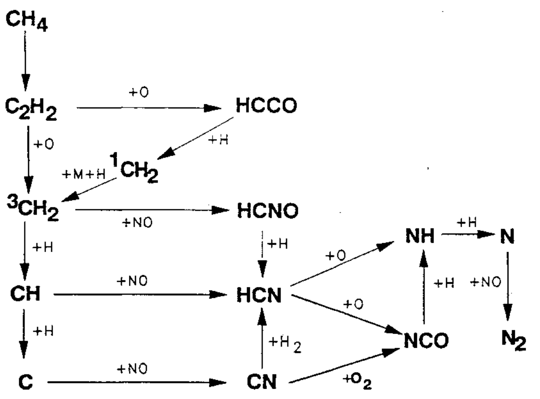


Fig. 3 Reburn reactions.

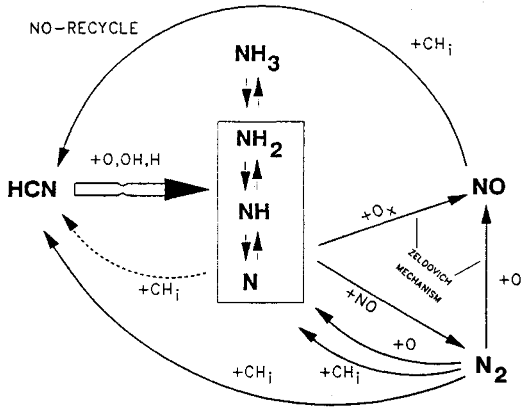


Fig. 4 Nitric oxide formation and destruction in flames.

cipal factor in the control of NO_x formation, as this determines the local oxygen concentration, radical species, the rate of release of hydrocarbon (and fuel nitrogen) species in the critical areas, and subsequent local flame temperature. By controlling the rate of fuel and air mixing (i.e., straining of the fuel into the surrounding air), the individual burners can be designed to minimize the formation of NO_x. In all cases the local temperatures are far from those of stoichiometric fuel/air mixtures. Some design concepts use fuel-rich zones which inhibit NO_x formation. In general, typical low NO_x burners have multiple air channels with provisions for controlled fuel and air mixing. Proportioning of the combustion air between the various channels is achieved by carefully tailored burner geometry. Alternatively, fuel could be distributed in stages.

Variable air swirl, e.g., by using a variable geometry swirl combustor,[3,4] can be used to control both the initial fuel-air mixing and the structure of the flame close to the swirler exit. These techniques have generally been grouped together as air staging. Alternatively, fuel staging can also be used. Many examples exist, particularly for stationary gas turbines, that incorporate fuel staging in the fuel nozzle design. Fuel staging introduces a series of fuel-rich streams into the critical flame region for reducing NO_x. In contrast to the conventional emphasis on temperature, controlled flame chemistry provides an important role on NO_x formation and emission.

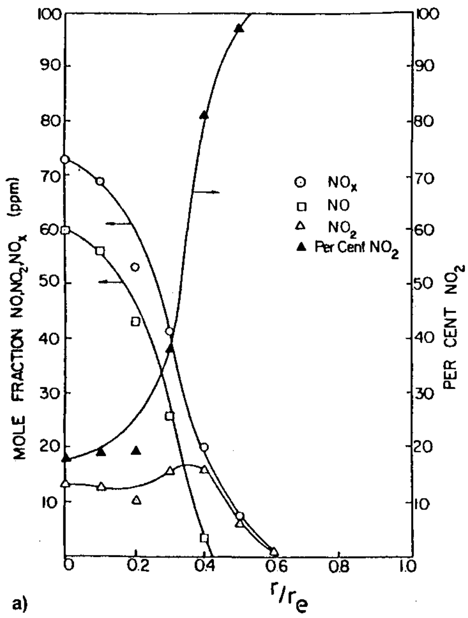
The formation rate of nitric oxide from fuel-bound nitrogen is only slightly dependent upon temperature,[9] and increases markedly with increased oxygen concentrations. Different forms of fuel-bound nitrogen have a significant influence on the conversion to nitric oxide. Low boiling point additives provide low yield as compared to high boiling point additives of nitrogen.[5] Increasing fuel nitrogen increases NO_x emissions, but the conversion efficiency decreases.[6] Experiments carried out on premixed and diffusion flames show a decrease in conversion efficiency with an increase in equivalence ratio.[6–8] The reduction is particularly significant under fuel-rich conditions. Therefore, control techniques such as flue gas recirculation, which aim at lowering the combustion temperature, have little effect on fuel nitrogen conversion. The different mechanisms and their practical approaches used in industry for thermal and fuel de-NO_x are given in Ref. 6.

IV. NO_x Reduction to N_2 During Combustion and its Conversion to NO_x

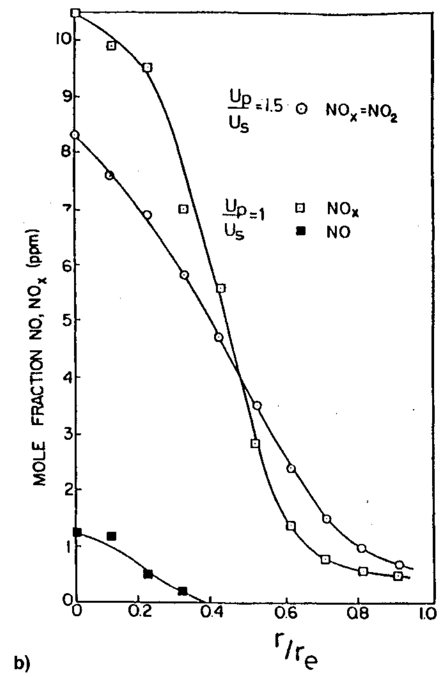
The destruction of NO has been observed via controlled chemistry and/or mixing in flames.[10–20] The prompt NO formation rate has a positive pressure dependence[9] and provides small contribution relative to thermal and fuel NO_x under flame temperature conditions. These studies support the additional need for developing combustion systems having series of fuel-rich zones followed by lean zones, or those having very lean premixed fuel-air mixtures.

Local NO formation rates were studied from experimental data obtained in a diffusion-type, natural gas-fired swirl burner.[10] Evidence of NO destruction in the recirculation zone was also found. The effect of fluctuating temperature on the rate of NO formation in the flame was carried out for evaluating the departure between calculated and experimental results. The effect was significant, but did not allow the large discrepancy between experimental and calculated results.[10]

The amount of NO_2 in NO_x can be quite significant under certain conditions.[21,22] The effect seems primarily to be due to rapid quenching processes in the burner and is thought to be formed via NO oxidation by HO_2 free radicals. Radial variation of NO_x, NO, NO_2, and percent NO_2 at a position six diameters downstream of the combustor inlet under co-swirl flow conditions are shown in Fig. 5a. NO_2 is formed nearly uniformly across the central section of the burner, and has a small peak at the interface between the primary and



a)



b)

Fig. 5 Pollutant emission characteristics with methane flames.[4] Primary air swirl = 0.523, secondary air swirl = ±0.559, primary airflow velocity = 35 m/s, and secondary airflow velocity = 23.3 m/s: a) co-swirl and b) counterswirl.

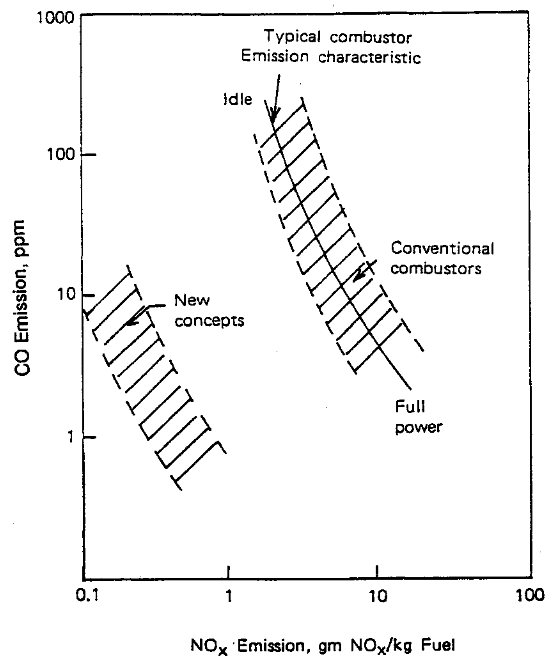


Fig. 6 Emission characteristics of conventional and advanced combustors.[24]

secondary flows where quenching effects are maximized. Introduction of counterswirl provides higher levels of NO_2 in NO_x as compared to the co-swirl case for both velocity ratios (Fig. 5b). Rapid mixing of the two flows in the counterswirl case provides flame quenching and dilution. This yields little or no NO formation. The complex reaction between the fluid dynamics of the flow and active chemical species provides relative proportions of NO and NO_2. Recently, Gupta et al.[22] reported the important effect of a combination of co- and counterswirl flames on NO and NO_2 emission using a variable geometry swirl combustor. The results show that straining of fuel and its proper injection into the shear layer, obtained by a suitable combination of fuel injector and burner geometry, significantly influences the NO_x emission levels.

NO_2 emission from gas turbine combustors increases exponentially with flame temperature (NO_x generation proportional to $e^{0.009T}$), other parameters being important only insofar as they affect the flame temperature.[21,23] Elimination of "hot spots" from the reaction zone helps NO_x reduction.

A basic feature of nearly all methods of emissions reduction is that they represent "tradeoffs" between carbonaceous particulates—CO, and unburnt hydrocarbons (UHC) on one hand, and NO_x on the other. This point is illustrated in Fig. 6 which shows the CO vs NO_x emissions for a typical gas turbine combustor.[24] For any given combustor the CO/NO_x emission characteristic remains sensibly constant, with the upper and lower extremities of the curve corresponding to operation at idle and full power, respectively. The main advantage to the designer in most of the emission reduction techniques described below is in allowing movements along the curve over and above those dictated by changes in engine power setting. Nevertheless, real progress in emissions technology is achieved only by displacement of the CO/NO_x characteristic nearer to its origins using advanced combustion concepts.

V. Development of Low NO_x Combustors

The development of low NO_x combustors is proceeding along two main lines. The most direct approach is through various minor modifications to conventional designs, for example 1) by changes in liner geometry and airflow distribution; 2) by the adoption of more sophisticated methods of fuel injection; 3) by the practical exploitation of maintaining the combustion history farther away from stoichiometric conditions; 4) by maintaining low levels of temperature fluctuations; and 5) new wall-cooling techniques that are more economical in their use of cooling air.[21]

The merit of this approach is that the combustor retains its existing general size and configuration, and improvements can be made without trespassing far outside the bounds of established technology. Its main drawback is that the end product must inevitably be a compromise of some kind in regard to emissions and other aspects of combustion performance.

The other approach is essentially a rejection of the present design philosophy, which is based on heterogeneous diffusion flames and is fairly conservative in its distribution of fuel and air. Of the various advanced concepts now being actively studied, the four most promising appear to be variable geometry; staged combustion; e.g., rich burn, quick quench, lean burn (also called the RQL) combustor; lean premixed prevaporized (LPP); and catalytic oxidation. All of these options are presently being persued under high speed research (HSR) low NO_x program for use in high speed commercial transport (HSCT). Low NO_x potential of gas turbine engines is given in Ref. 25. The challenges associated with HSCT development are given in Ref. 26.

Advanced concepts may include some combination of co- and counterswirl arrangement into the combustor which allows one to control the precise flame behavior via fuel nozzle design and air swirl and its distribution. This approach of fuel straining as well as the availability of rich radical pool species for destructing NO within the flame zone has enormous potential for low NO_x combustor development.

The present concern of HSR emissions programs is on nitrogen oxides (NO_x) which, through a series of known catalytic reactions, could adversely impact the Earth's protective ozone layer. Although continuing atmospheric studies are needed to fully understand and quantify the levels that would yield no damage, it is clear that technology development focused on reducing NO_x emissions is paramount before U.S. industry could commit to a high-speed transport development program. A presently ongoing emissions reduction program indicates that reduction to levels in the range of 3–8 g of NO_x per kilogram of fuel burned is possible with advanced combustor design approaches. Further NO_x reduction and potential elimination may also be achievable through secondary means such as downstream (postcombustion) injection of chemical reactants. The goals of the HSR program on advanced combustor technology for NO_x reduction and engine fuel efficiency gain are given in Fig. 7. Included in this figure is the best available current cumbustor technology. The goal is to achieve an NO_x emission index of 5 gm/kg of fuel. In the RQL approach the first stage is operated under fuel-rich conditions (mixture equivalence ratio limited by smoke formation) followed by a fuel-lean burning second stage. Correlations are available for this index. Typical HSCT supersonic cruise combustion operating conditions are: T_{in}: 1000–1300°F; P_{in}: 12–14 atm; T_{exit}: 3000–3400°F; fuel: Jet-A (thermally stabilized jet fuel, TSJF).

Successful development of low NO_x combustor technology for supersonic transport engines poses a significant set of challenges. The first relates to the need for substantial fuel efficiency gains to achieve viable aircraft performance and economics. The gains dictate considerable increases in the engine's combustor pressure and temperature environment, which accentuates the potential for NO_x formation, e.g., the NO_x level could double or triple relative to concorde-type technology, if not specifically controlled. This requires a departure from current combustor designs using high-temperature primary zones (near stoichiometric conditions), toward advanced designs based on fully premixed, two- or multistage approaches that constrain peak temperatures to very near the average combustor exit temperature. With most development and operational experience of these approaches, limited to ground-based applications, the advanced designs must also continue to meet unique aircraft-engine operating requirements such as rapid power transients and altitude relighting. The planned program aggressively pursues solutions to all of these challenges.

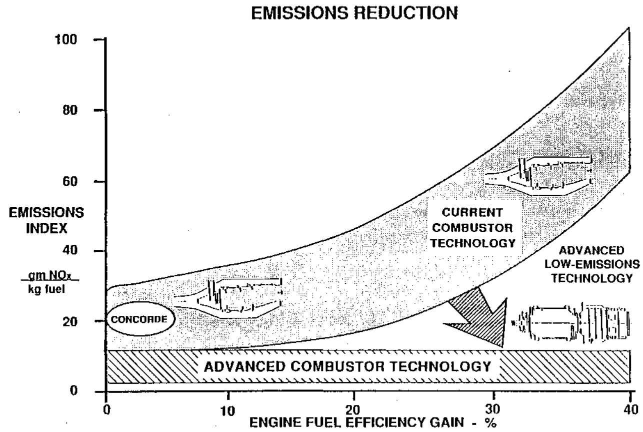


Fig. 7 NO_x emissions index vs engine fuel efficiency gain of current and advanced combustors.[26]

VI. Catalytic Combustion

An argument against the use of the simple two-stage combustor is that, in designing to achieve rapid mixing of first-stage products and second-stage air, reactions could well be quenched, and the combustor could operate at low efficiencies with subsequent HC and CO pollution. Alternatively, if the air injection in the second stage is too slow, local high-temperature regions might well give rise to excessive temperatures with the formation of substantial quantities of thermal NO_x.

The use of a catalytic second stage is an attempt to overcome these objections. The first stage remains as it was in the simple two-stage combustor. This is immediately followed by a dilution zone where every attempt is made to quench any reaction rapidly. Thus, the gases entering the second-stage catalytic region are in weak conditions, and combustion is completed at very low reaction temperatures, thereby obviating the formation of thermal NO_x.

The catalytic version would require special attention to the design of the first stage, since it is unlikely that any soot formed in this zone could be burned within the catalyst bed. In fact, it is probable that soot deposits would reduce the efficiency of the catalytic section and perhaps cause blockage.

Probably any two-stage combustor will have to function as one or more stirred reactors. The effect of the pressure loss upon stirred reactor performance has been studied by Odgers,[27] and it was found that, below 3% pressure loss, the falloff in performance was spectacular. Hence, it is tentatively suggested that a minimum wall pressure loss of about 5% should be expected for a two-stage combustor. A possible exception to this is that industrial combustors using an exterior supply of fuel "blast" air might well produce sufficient stirring within the present low-loss configurations.

The two-stage catalytic combustion as proposed by Krill et al.[28] utilizes two catalytic stages, separated by an interstage heat exchanger, the first stage being fuel rich. For gas turbine application, the interstage heat exchanger would be removed and the second-stage temperature control would be achieved by dilution with excess air. A test of this system (using NH_3 as "fuel" nitrogen) showed that as little as 10% of the fuel nitrogen was converted to NO_x, compared with an 80% conversion for simple combustion. The following results are significant[28]:

1) The two-stage combustor is effective in controlling conversion of fuel nitrogen to nitrogen oxides under stoichiometric and fuel-lean conditions.

2) The variation of first-stage stoichiometry impacts overall fuel nitrogen conversion.

3) First-stage sooting of the cobalt oxide catalyst was a limiting factor in combustor operating life.

Application of the concept to turbine systems is possible. Research is underway in some of these areas.

VII. Alternative Fuels

Finite resources of fossil fuels will eventually be depleted and it is expected that alternative fuels will provide greater application in various propulsion systems. It is also expected that petroleum fuels will be utilized more for materials production rather than energy conversion. The combustion of alternative fuels (synthetic fuels, synfuels) is expected to be complicated by the presence of high carbon to hydrogen atomic ratio, and high nitrogen, sulfur, and aromatic content in the fuel, which results in the increased emission of soot, NO_x, carcinogenic polycyclic aromatic hydrocarbons, increased combustor liner heating, and increased ignition time.[29-33]

The formation of soot in practical equipment is correlated better by the hydrogen content of the fuel than the analysis for total aromatics, since individual aromatics vary considerably in tendency to form soot and, also, in hydrogen content. Napthalene is well known to produce considerably more soot than butyl-benzene (both containing 10 carbon atoms), and to provide a correlation with percent hydrogen. The fuel characteristics most likely to affect the design of future gas turbines are fuel C/H ratio, viscosity, volatility, nitrogen content, and fuel stability. The use of high C/H ratio fuels increases the kinematic viscosity, surface tension, specific gravity, and the amount of soot produced. These changes in fuel properties have an adverse impact on the atomization quality of the spray when a given fuel injector is used. Increased number of carbon particles formed in fuel-rich regions of the primary zone lead to higher liner temperatures and higher smoke emissions. Reduced volatility and increased viscosity affect droplet lifetimes and atomization, respectively. Volatility affects the rate of fuel vaporization in the combustor can. Since important heat release processes do not occur until gas-phase reactions take place, a reduction of volatility reduces the time available for chemical reaction within the combustion system. In the aircraft engine this can lead to difficulty in ground- or altitude-ignition capability, reduced combustor flame stability, increased emissions of CO, hydrocarbons, and the associated loss in combustion efficiency. Moreover, carbon particle formation is aided by the formation and maintenance of fuel-rich pockets in the hot combustion zone. Low volatility allows rich pockets to persist because of the reduced vaporization rate. Increased soot causes additional radiative loading to combustor liners.

The desired formation of a finely dispersed spray of small fuel droplets is adversely affected by viscosity. Consequently, the shortened time for gas-phase combustion reaction and the prolonging of fuel-rich pockets experienced with low volatility can also occur with increased viscosity. Ignition, stability, emissions, and smoke problems also increase for higher viscosity fuels. Increased fuel-bound nitrogen in alternative fuels leads to increased NO_x emissions. Methods used to reduce NO_x from petroleum fuels can be used here for NO_x reduction. The mathematical modeling of combustors using alternative fuels requires unique challenges.[34,35] The use of alternative fuels in combustors would require not only the redesign of liners, but the whole combustor so that emissions and soot production can be controlled.[36]

The amount of carbon produced is very dependent upon fuel composition, pressure, and operating conditions. Fuel structure has a significant effect on the sooting tendency of diffusion flames, but little influence in premixed flames.[37] Irrespective of the fuel type in diffusion flames, soot inception occurs around 1400 K and is dependent somewhat on H atom diffusion. Soot particle burnout ceases at about 1300 K.[37] The trend for various fuels observed the order: aromatics > alkanes > alkenes > alkynes.[37] As an example, benzene was found to have a greater tendency to soot than ethene or acetylene. For diffusion flames however, the trend is aromatics > alkynes > alkenes > alkanes. For gas turbine combustors the soot content may be evaluated from hydrogen content and the ratio C^*, where

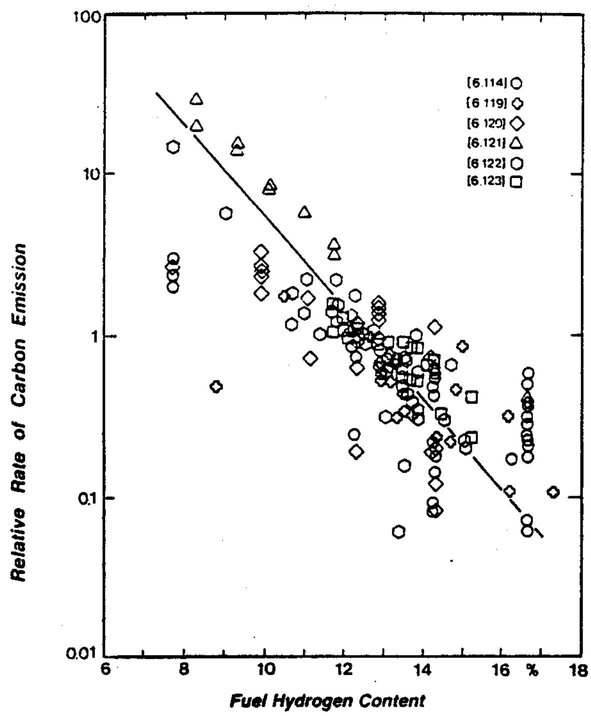


Fig. 8 Effect of hydrogen content on carbon emission in various combustors.[29]

$$C^* = \frac{\text{carbon formed by any fuel}}{\text{carbon formed by a fuel having 12.5\% hydrogen}}$$

The carbon emission index is then evaluated from

$$EI_{\text{carbon}} = 1.08 \times 10^{-29} \left(\frac{p}{O/C}\right)^{2.7} (H/C)^{-5.45} T_o^{-8.66}$$

The effect of hydrogen content on carbon emissions in various combustors is given in Fig. 8. Changes in fuel preparation, inlet temperature, pressure, or primary zone equivalence ratio would alter the results.

The cost of cryogens is the key deterrent toward their use in commercial transport. The most optimistic basic costs for hydrogen and methane are higher than the current price of conventional jet fuel (jet A). In addition to the basic cost of fuel, cost penalties must be added for ground and aircraft vaporized fuel losses and for construction of new airport distribution, storage, and aircraft servicing equipment. Some challenges and experience with hydrogen and other alternative fuels, including the commercial flight demonstration with hydrogen, are given by Sosounov.[38]

VIII. Endothermic Fuels

The development of endothermic fuels which are capable of absorbing the aerodynamic heat generated by aircraft operating in the Mach 3 to 6+ range (e.g., HSCT application) is extremely important. The desired fuel will absorb the heat by virtue of its sensible and latent heat and its endothermic reaction capability.[87] This in turn requires the fuel to have excellent thermal stability up to its reaction temperature and then react rapidly and cleanly to yield products which serve as exothermic fuel for the engines. The general feasibility of these fuels is now well underway but many technical details as to the specific application still remain to be examined. The particular fuel selected for the aircraft cooling system must transfer the heat generated by several sources in a desired manner. The major effort now is to determine the factors which can modify the distribution of heat sink capacity over the available temperature range. The significant factors are the type of fuel (e.g., paraffinic, napthenic, or mixed, etc.), the type of endothermic reaction to be performed (e.g., cracking, dehydrogenation, dehydrocyclization, depolymerization), storage, contaminants, additives, and the means of carrying out the reaction (e.g., thermal, catalytic). Combustion via the vaporizing and endothermic principles means that the exothermic fuel will be fed into the engine in the form of fuel vapors having different molecular weight species. As an example, absorption of heat by methylcyclohexane (MCH) in the presence of a catalyst produces hydrogen and toluence. The density and heat of combustion of MCH are 48.3 lbm/ft^3 and 19,350 Btu/lbm, respectively, and are very similar to that of JP7 fuel. The properties of this fuel will be significantly different from that present in the main fuel tank. The dehydrogenation of napthene results in the formation of hydrogen and aromatics. Continued cooperation between federal agencies, government labs, engine and mainframe manufacturers are serving to bring various aspects of the problem into sharper focus. Efforts to accumulate additional information and opinions are expected to grow in the future. Considerations of times, temperatures, and volumes which can be expected in supersonic/hypersonic aircraft have led to some tentative conclusions with respect to the operational use of endothermic fuels in high-speed aircraft. Some endothermic fuels have shown heat absorption capacity in excess of 2000 Btu/lbm under simulated flight conditions. Some of the presently ongoing research is in the area of reaction studies, design parameters and thermal stability.

IX. Nonintrusive Diagnostic Techniques

Many of the presently exploited diagnostic techniques are not new and the use of optical diagnostics in combustion research dates back to 1857, when the C_2 emission from flames was observed. The elastic scattering of light to explain the blue color of the sky was given by Lord Rayleigh in 1871. The availability of laser provides the examination of very weak processes which were not practical previously. Laser velocimetry and droplet/particle sizing techniques are now extensively used in many practical combustion systems.[18,89] The miniaturization of laser-velocimeter and particle-sizing equipment for simultaneous measurements of three velocity components (and shear stresses) and particle size will continue to develop in the 1990s. Although the phase-Doppler analyzer has provided significant advances in particle sizing the response of the system over a large dynamic range, system gain sensitivity on particle size, system miniaturization, and spectral information will continue to be on the priority list. Laser-based diagnostic techniques have also been used to provide spatially and temporally resolved information on temperature, concentration, etc., in both laboratory size flames and practical combustion systems.[90,91] Future efforts are expected to focus on obtaining correlations between two and more quantities in addition to better accuracy and precision of the system, frequency response, system miniaturization, ease of operation and reduced cost.

X. Combustion Modeling

Practical combustion systems incorporate interdependent phenomena of three-dimensional multicomponent flowfields with complex multiphase chemical kinetics, evaporation, and heat transfer processes, all occurring simultaneously. Requirements include improved simulation of the combustion processes, with particular emphasis on fluid dynamics and modeling. The lack of understanding of the internal behavior is not surprising. Consider, for example, that the combustor flow is two-phase (liquid fuel and air) and includes some of the most formidable technical challenges in fluid dynamics (turbulence, variable density, elliptic flow), heat transfer (conduction, convection, and radiation), thermodynamics (varying composition), and chemistry (high-temperature kinetics). Nonetheless, for combustor technology to advance, an improved understanding of these processes is required. Applied combustion research needs to include the clean and efficient combustion of fossil fuels and future low-grade liquid and solid fuels, and the associated reduction of pollution through combustion control. Fundamental combustion research needs to be done in the areas of interactions between turbulence and kinetics, computer model development, gas and solid phase kinetics, droplet/particle cloud combustion, soot formation and chemistry, and flame structure. Extensive descriptions can be found relating to swirl flows,[4] flowfield modeling and diagnostics,[18] gray areas of combustion,[39] and related studies by Lilley and colleagues.[40–44] References 43 and 44 relate to studies concerned with the aerodynamics of mixing in typical combustors. Other work is summarized in Ref. 45, where the focus is on the assessment, development, and application of combustor aerothermal models.

The field of combustion is diversified by the complex nature of most reaction processes. Fuel chemistry, fluid mechanics, convective and radiative heat transfer, gas-phase elementary reactions, turbulence, and particle kinetics and dynamics are relevant processes that often have a direct and sometimes controlling influence, on the behavior of a particular combustion system. In combustion systems the designer must accomplish efficient and pollutant-free combustion economically in which turbulent reacting multiphase swirling flow occurs. In design situations, experimental data is used to verify and develop models. These mathematical models then supplement and reduce the amount of costly and time-consuming experimental procedures. These models bring benefits and entail costs. Benefits include knowing quantitatively, in advance, what will be the performance of equipment which has not yet been built, or which has not yet been operated in the manner under investigation. Most mathematical models simulate the physical processes (for example: turbulence, radiation, combustion, pollutant formation, and multiphase effects) by solving an associated set of coupled partial differential equations. Related recent textbooks include Refs. 46–56, while Ref. 39 includes some of the significant reviews related to the prediction of combustion flowfields.

The ultimate goal has been to develop a reliable combustor design system that can provide quantitatively accurate predictions of complex combustion flowfield characteristics so that an optimum combustion system design can be achieved within reasonable cost and schedule constraints. The rapidly developing computational fluid dynamics (CFD) capability is providing an additional tool in the design process which can have a powerful positive influence on future design capability. In these codes, combustion system subcomponents including diffusers, fuel injectors, and combustor liners, in addition to the complex internal flows, need to be accurately modeled.

To achieve this, physical submodels and accurate numerical schemes must be developed to describe the various aerothermochemical processes occurring within the combustion chamber. A very extensive assessment of numerics, physical submodels, and the suitability of the available data was made by three contractors under Phase 1 of the HOST Aerothermal Modeling program.[57–59] These investigations surveyed and assessed current models and identified model deficiencies through comparison between calculated and measured quantities. Results of the assessment by Srinivasan et al.[59] included 1) simple flows with no streamline curvature, 2) complex flows without swirl, and 3) complex flows with swirl. Geometries for several test cases from each of these categories are summarized in

Ref. 45. The major conclusion of the HOST Aerothermal Modeling Phase I assessment studies was that the available CFD codes provided a useful combustor design tool. Although significant advances have been made in the development and validation of multidimensional gas turbine combustion calculation procedures, the codes assessed were only qualitatively accurate, especially for complex three-dimensional flows, and further work was needed. It was concluded that both a significantly improved numerical scheme and fully-specified experimental data (i.e., both mean and turbulence flowfield quantities with measured boundary conditions) for complex nonreacting and reacting constituent flows were needed before various emerging physical submodels of turbulence, chemistry, sprays, turbulence/chemistry interactions, soot formation/oxidation, radiation, and heat transfer could be properly assessed.

The first-generation combustor design procedure outlined by Mongia and Smith[60] has been very useful for developing several combustors (Mongia et al.[61]) that exhibited significant technology advances. However, in addition to the model deficiencies identified in the assessments, there were several parameters of importance in gas turbine combustor design that the analytical models could not predict. For example, gaseous emissions, soot formation, flame blowout limits, combustor pattern factor, and liner heat transfer. These parameters were, however, successfully predicted by well-established semianalytical correlations developed by Plee and Mellor,[62] Lefebvre,[63] and their associates.

Therefore, a combustor design procedure that could be applied to current and future gas turbine engines was implemented that makes use of empirical design concepts and employs analytical modeling tools to represent various combustion processes (see Rizk and Mongia[64] and Mongia[65]). This method makes use of multidimensional models to establish liner flowfield features and combustion characteristics. The analytical results are then integrated with semiempirical correlations for performance parameters of interest. That is, flowfield and geometric parameters that are needed in the empirical equations, such as combustion volume and the fraction of air participating in the primary combustion reaction, are provided by the analytical calculations.

Based on the recommendations of the Phase I assessment studies, activities in Phase II of the HOST Aerothermal Modeling program concentrated on developing improved numerical schemes, and collecting completely specified data for nonreacting single and two-phase swirling and nonswirling flows. The programs initiated were: Improved Numerical Methods; Flow Interaction Experiment; and Fuel Injector/Air Swirl Characterization. The programs are summarized by Holdeman et al.[45] Information of the type being sought in these programs (and others) is not only insightful, but provides a valuable data set for the development and verification of comprehensive codes under development for advanced combustor design. The interested reader may consult further studies about developments in turbulence,[92] reacting flows,[93] heat transfer,[94] propulsion,[95,96] and pollution reduction strategies.[97,98]

XI. Numerical Simulation

The computational solution of two- and three-dimensional flowfield problems entails the solution of many simultaneous nonlinear equations, including up to three velocity components, pressure, stagnation enthalpy, turbulence quantities, and species concentrations. Since the equations are all similar in form, the same solution algorithm can be used for all of them. Problems are classified according to their dimensionality (the number of independent variables from three space dimensions and time) and type (parabolic or elliptic). The flow classification of parabolic [possessing one coordinate direction with first-order but without second-order derivatives—boundary layer type with prominent direction(s)], or elliptic (possessing second-order derivatives in all coordinate directions—recirculating type with upstream influence), governs the type of boundary conditions required and the method of solution. Marching methods are appropriate for the former and relaxation methods for the latter. The problems, methods, solution procedures, and typical sample calculations together with a comparison with available experimental data are discussed in swirl flow modeling studies, see Refs. 4 and 18.

The essential differences between the various computer codes include the complexity of the equation set for the simulation of the physical processes, the storage requirements, the location of variables in the grid-space system, the method of deriving the finite difference equations that are incorporated, and the solution technique. In primitive pressure-velocity variable formulations, a staggered grid system normally is used. In computational fluid dynamics, the "best" representation of the convection and diffusion terms is essential to the accuracy and convergence or stability of the interaction scheme or marching procedure. At high cell Reynolds numbers, a certain degree of "upstream differencing" is often used for a more accurate representation of the advection terms, including recent skew and/or weighted upstream differencing practices. Solution procedures vary from Gauss-Seidel point methods to more efficient line-by-line semi-implicit method for pressure-linked equations (SIMPLE) methods for steady-state problems, with corresponding explicit and SIMPLE methods for associated transient problems. Special techniques are available for the inclusion of detailed chemistry into the solution schemes. Useful textbooks in this field include Refs. 66–69.

More accurate simulations of the combustion process are emerging, with inclusion of flowfield structures and turbulence, radiation heat transfer, and carbon monoxide and nitric oxide prediction. The governing equations are nonlinear and must be solved simultaneously, giving the numerical analysis of reacting flow problems its peculiar difficulty and flavor. The similarity between the differential equations and their diffusional relations allows them all to be put in a common form and solved in a similar manner. Related numerical studies include Refs. 70–76 and the wealth of information given about the "gray" areas of combustion research, see Ref. 39. It is propitious to be aware that several commercially available computer codes are available that solve fully three-dimensional combustion problems with advanced simulation models included. Some of these are reviewed in Refs. 77–80. Significant computer simulations have emerged from recent studies carried out in academia, government laboratories, and industries. These studies have provided much understanding of the complex problem and aided to the design of low-emission combustors. The development of advanced numerical techniques which can be applied with advantage to turbulent recirculating reacting flowfields include, error reduction program, application of improved numerical schemes, numerical modeling of turbulent flows, advanced numerics for multidimensional fluid flow calculations, and grid flexibility and patching techniques. A consensus of results indicated specific needs in future research studies: 1) improved finite-difference representation (with versions of bounded skew upwind differencing and/or other techniques); 2) faster convergence techniques via improved numerical solution schemes; 3) improved domain simulation (with boundary-fitted coordinate systems, or orthogonal grids, finite element methods, etc.); 4) more accurate hot-gas heat-transfer input; and 5) improved turbulence and turbulence/chemistry treatment.

There is a need to determine and incorporate new finite difference schemes and/or error reduction techniques into currently existing computer code models. Improvements in the accuracy of representation (differencing schemes) and rapidity of convergence (solution algorithms) are being sought before computer codes can give quantitative, rather than qualitative, predictions. Better numerics, improved understanding of inlet flow, improved turbulence modeling, and improved understanding of unsteady problems are required. Techniques for improved accuracy (including several bounded versions of skewed upwind differencing), improved versions of the pressure-velocity coupling technique, and methods for speeding convergence of iterative procedures are needed. A significant deficiency identified in the earlier assessments (see Refs. 57–59) was that, for many flows of interest, the accuracy of the calculation was limited by the numerical approximations, wherein the false diffusion is of the same order of magnitude as the turbulent diffusion. This masked the differences between turbulence models such that very different models gave essentially the same result, and sometimes resulted in undeservedly good agreement between data and predictions. If false diffusion is present, the numerical solution obtained for any given flow depends on the grid density and distribution. The hybrid finite differencing scheme employed in generally available combustor codes can give excessive numerical diffusion errors which might preclude accurate quantitative calculations.

Three significant HOST programs had the primary objective to identify, assess, and implement improved solution algorithms applicable to analysis of turbulent viscous recirculating flows. Both solution accuracy and solution efficiency were addressed (see Refs. 81 and 82). For most practical problems, a central-differencing scheme would be ideally suited if it were unconditionally stable. Central differencing is a simple second-order scheme which is easy and straightforward to implement. However, for grid Peclet numbers larger than 2, central differencing can lead to over- and undershoots, and is unstable. The hybrid (central/upwind) scheme is stable for all Peclet numbers, but suffers from excessive false diffusion. An alternative scheme, named controlled numerical diffusion with internal feedback (CONDIF)[83] has unconditionally positive coefficients and still maintains the essential features of central differencing and its second-order accuracy. Another advanced numerical scheme, called flux-spline,[84] is based on a linear variation of total flux (convection + diffusion) between two grid points. This is an improvement over the assumption of uniform flux used in hybrid schemes, and leads to reduced numerical diffusion. Both of these schemes have been used to solve a variety of analytical, two-dimensional laminar, and turbulent flows. An attractive feature of both CONDIF and flux-spline schemes is that their extension to three dimensions is relatively straightforward. The resulting linear differential equations involve only 7 points as opposed to 27 points needed in many skewed-upwind schemes (Syed et al.[85]).

There is also a need for improved computational efficiency for a given level of accuracy. Typically the continuity and momentum equations are solved separately, and then linked through iteration of the pressure, see for example methods based on the semi-implicit method for pressure linked equations (SIMPLE) algorithm. Modifications, such as SIMPLER, SIMPLEST, and PISO, have been shown to improve computational efficiency. Other advances schemes (see HOST[81] and Vanka[86]), such as block correction techniques and direct solution of the coupled equations have been proposed. Calculations with the latter coupled with the flux-spine technique have shown a speed increase by a factor of 15 for a calculation of turbulent flow over a backward-facing step, see Ref. 65. Further discussion is given in the references regarding recent studies and application of multigrid solution methods,[99–104] differencing schemes,[105–109] convergence improvement,[110] and related applications.[111–114]

XII. Vision for the 1990s

The nineties will have greater attention on both environmental pollution and energy conservation. Advanced concepts for environmental pollution control require detailed understanding of the physical and chemical processes that undergo during combustion. Test data on laboratory-scale, bench-scale, and prototype are urgently needed for determining the details of the chemistry involved, fuel/air mixing, fuel injector design, combustor geometry, combustion air swirl, and flow distribution. It is expected that future combustors will be even shorter than they are today and the use of advanced fuels will require a closer look at the current design philosophy. Some of the alternative fuels have significant differences in fuel properties and combustion characteristics. Advanced new technologies will require some tradeoff between fuel availability and its properties, energy conservation, efficiency, and environmental pollution control. The use of endothermic fuels may provide attractive benefits for some applications. The development and use of laser diagnostics will continue to grow. This systematic approach involves online computer-based data acquisition at high frequency which provides information needed for theoretical model validation and model development. It is a challenge to handle the environmental problems, with low pollution from difficult fuels. It is an exasperating challenge for combustion engineers to handle the emerging environmental problems, achieve high efficiency, and conserve energy. Future gas turbines are expected to operate at even higher temperatures. This will provide further challenges in the area of liner cooling and materials. These problems are expected to be compounded by the use of low-grade fuels which are known to provide higher luminosity flames (presence of higher level of carbon particles) and result in greater radiation heat transfer. Computer hardware and software improvements will provide greater insight than ever before, this trend will grow further as computer power and numerical algorithms become more available to combustor developers and researchers. The theoretical contribution, together with advanced computer graphics, will grow in the nineties to further reduce the excessive time and cost of experimentation. The design and development of gas turbine combustion will truly become a science.

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