AEDC-TR-73-163

Cy Xerox

FG Conf Room

A LITERATURE REVIEW ON TURBINE COMBUSTOR MODELLING AND EMISSIONS

I. T. Osgerby
ARO, Inc.

November 1973

Approved for public release; distribution unlimited.

ENGINE TEST FACILITY
ARNOLD ENGINEERING DEVELOPMENT CENTER
AIR FORCE SYSTEMS COMMAND
ARNOLD AIR FORCE STATION, TENNESSEE

NOTICES

A LITERATURE REVIEW ON TURBINE COMBUSTOR MODELLING AND EMISSIONS

I. T. Osgerby
ARO, Inc.

FOREWORD

The work reported herein was conducted by the Arnold Engineering Development Center (AEDC) under the sponsorship of the Air Force Systems Command (AFSC), under Program Element 65802F.

The results of the research presented herein were obtained by ARO, Inc. (a subsidiary of Sverdrup & Parcel and Associates, Inc.), contract operator of AEDC, AFSC, Arnold Air Force Station, Tennessee. The research was conducted from July 1, 1972 through March 31, 1973, under ARO Project No. RD231, and the manuscript was submitted for publication on July 20, 1973.

This technical report has been reviewed and is approved.

EULES L. HIVELY
Research and Development
Division
Directorate of Technology

ROBERT O. DIETZ
Director of Technology

ABSTRACT

The rapidly growing body of literature on turbine combustor modelling is reviewed. The analytical models are presented and discussed with particular emphasis placed on their ability to predict gross operating characteristics as well as pollutant emission levels. Comparison is made between theory and engine and laboratory experiments showing the general inaccuracies of current models. A suggestion for improvement of the best available model is made, and areas for fundamental research are pointed out.

CONTENTS

ILLUSTRATIONS

TABLES

SECTION I
INTRODUCTION

This survey was written in an attempt to assess the status of turbine engine combustor research. There is a rapidly growing body of literature both on engine emissions test results and on analytical models of the combustion process. Prior to the mid-1960's, the majority of research reported was concerned with fundamental studies of combustion processes, and very little was published on the applications of this knowledge to practical engines. As shown by Gradon (Ref. 1), the development of an engine relied heavily on previous experience and a great deal of cut and weld modifications. At that time there was a growing emphasis on engine emissions, particularly with respect to visible soot and smoke (Ref. 2). The absence of a realistic analytical model of the turbine combustor process is adequately emphasized by the 465 combustor modifications and 140 full-scale engine tests carried out on the Pratt and Whitney JT8D fan engine to produce a smokeless combustor. The influence of the National Air Pollution Control and Administration (NAPCA) and the Environmental Protection Agency (EPA), Climatic Impact Assessment Program (CIAP) is being felt throughout the manufacturing industry and by users, both civilian and military. Research on automobile emissions has shown that hydrocarbons, nitric oxide, and sunlight lead to production of per-oxyacetyl nitrates (PAN) in smog (Refs. 3 through 5). Emission of carbon dioxide, steam, nitric oxides, and particulates at altitude has led to suggestions of a green-house effect, ozone depletion with increased cosmic ray penetration and increased sunlight reflection by particulates generating a new ice-age. Accurate assessment of the real emissions problem is essential. Required modifications to engines should be based on predictions of analytical models coupled with, rather than solely by, the cut and weld approach if they are to be accomplished at reasonable cost. Currently, analytical models are, at best, marginally adequate in predicting emission levels at cruise design point and inadequate in predicting gross operating characteristics such as blowout, relight, mixing rates, etc. It is suggested that an analytical model should first be capable of predicting all the gross characteristics accurately before pollutant emission predictions are made.

A typical turbine combustor can is shown schematically in Fig. 1. It is generally divided into three zones: primary, secondary, and dilution. The primary zone consists of a fuel injection region and a highly stirred reaction region. Combustion occurs at essentially stoichiometric fuel/air ratio (liquid hydrocarbons have very narrow flame stability limits) with approximately 90-percent combustion completion occurring in it. The secondary zone completes the combustion to about 99 percent and initiates dilution, completed in the dilution zone, to provide an acceptable turbine inlet temperature.

The turbine engine, operating near the cruise design point, has a very efficient combustor, and overall heat release rates can be predicted quite well (Ref. 6) assuming air is instantaneously mixed with fuel and burnt. However, performance at idle (minimum throttle setting, relatively low turbulence level) and takeoff (maximum throttle setting, relatively high turbulence level) are predicted rather poorly because of the different fluidynamics and chemistry interactions in the combustor at these throttle settings. A much more complicated model of the combustor is required, which considers locally fuel rich-fuel lean regions caused by incomplete mixing of fuel and air, and also considers the problems of blowout and relight. Recent research has shown that the combustor zones contain several distinct regions in which mixing rates are intense and some in which little mixing occurs. The phenomenon of hysteresis in the primary zone in which blowout occurs at a higher flow rate (shorter residence time) than can be tolerated for stable ignition can now be readily explained. Consider two high mixing rate reactor regions coupled by a zero mixing rate reactor (plug flow) which recirculates the products of one to the other. This additional reactor enables the high mixing rate reactors to boot strap each other in such a way that the combustion products of one helps to sustain the flame in the other. This model also indicates that raw fuel is subjected to flame temperatures in the individual reactors and, in particular, in the injector region. Thus, instantaneous mixing and evaporation does not occur (as implied in most analytical models) and a mechanism and conditions for thermal degradation (pyrolysis) of fuel to soot and hydrocarbon fragments obviously exist.

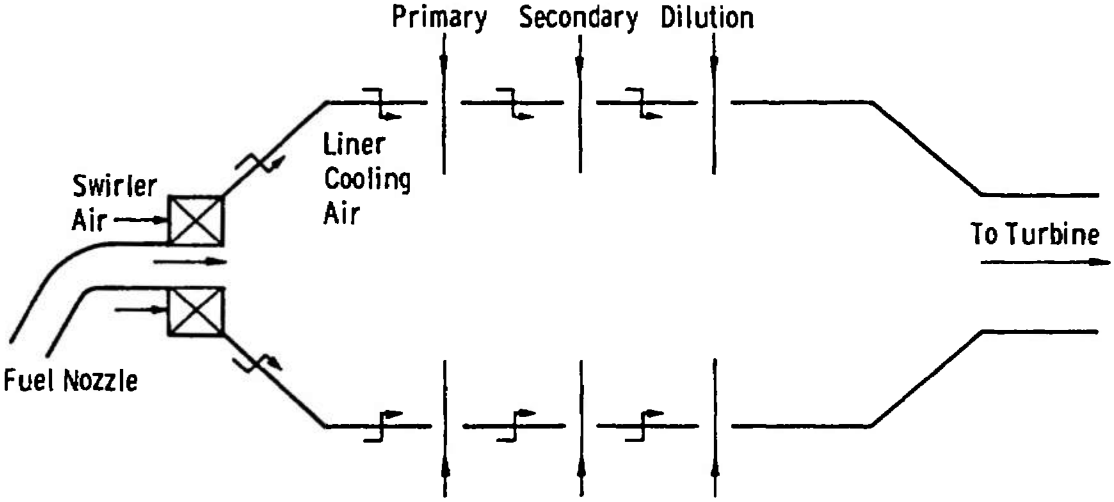


Fig. 1 Typical Turbojet Combustor Can

Current theoretical models (discussed later) are inadequate for predicting pollutant emission levels even at the cruise design point. Extensive data from turbofan engines (sea-level static tests) were presented in Ref. 7 and correlations of the data by Lipfert (Ref. 8) have shown that nitric oxide (NO_x) production is primarily a function of combustor inlet temperature and secondarily pressure (see Fig. 2). Additonal tests (Ref. 9) with extensive coverage of the engine exhaust plane with rakes and traversing probes have confirmed these correlations (Fig. 3a). A secondary parameter is specific humidity as shown in Figs. 3a through d and Table I, although the conclusions of Refs. 8 and 9 differ in the magnitude of its effect. Calculations by Edelman (Ref. 10) indicate that treating the primary combustor as a simple, perfectly stirred reactor (mixing complete on a microscale in a time << the residence time - typically one millisecond), and using current NO_x chemical reaction schemes, is inadequate to produce even qualitative agreement with engine emission data as shown in Fig. 4. Note that the curve was arbitrarily displaced to coincide with the match point and that the engine data curve is concave upward and the theory curve is concave downward. The qualitative influence of pressure, temperature, and residence time on NO_x production is shown in Fig. 5. The situation is quite dismal for prediction of soot and unburned hydrocarbons for which no rates are known. Lipfert (Ref. 8) has provided a means by which the latter can be estimated by correlating unburned hydrocarbons with carbon monoxide as shown in Figs. 6 and 7. This particular correlation is, however, limited to the class of engines investigated (for high bypass, high pressure, turbofans) as is the improved version of Ref. 9 (see Fig. 3d). A different correlation can be expected for different engines as evidenced by the different correlation for low pressure, turbojet engines (Refs. 11 and 12).

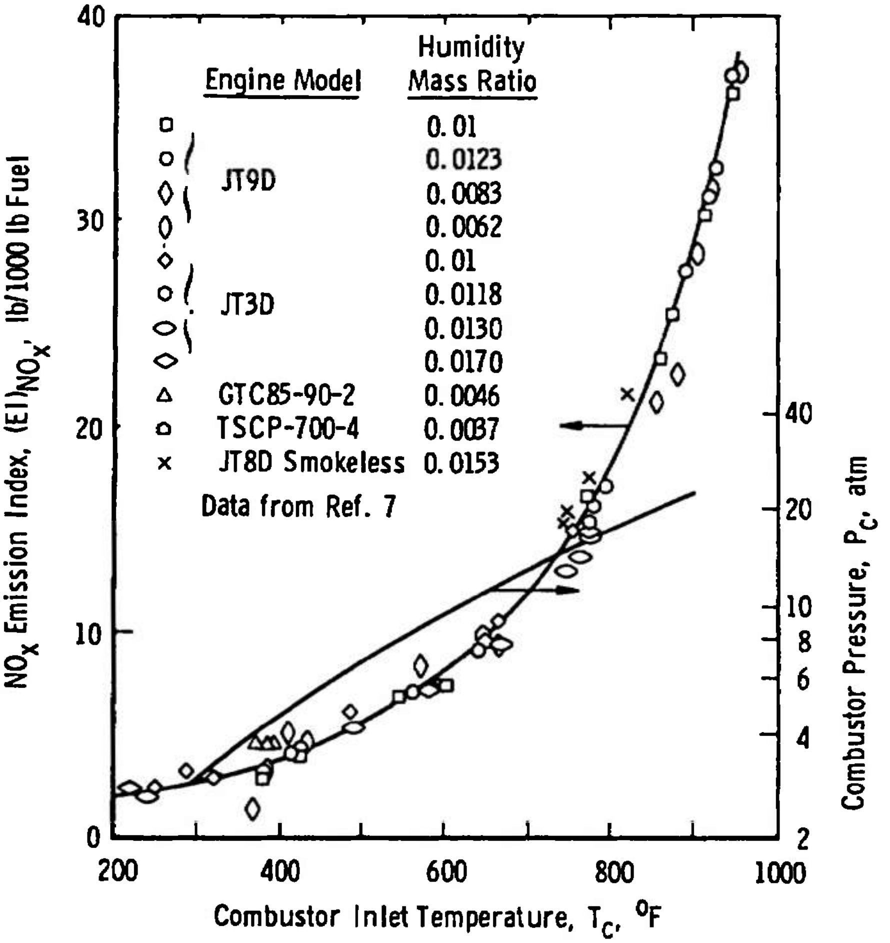
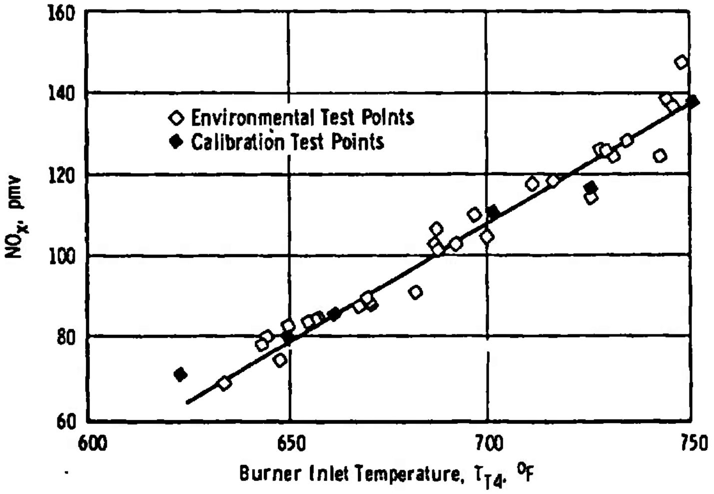
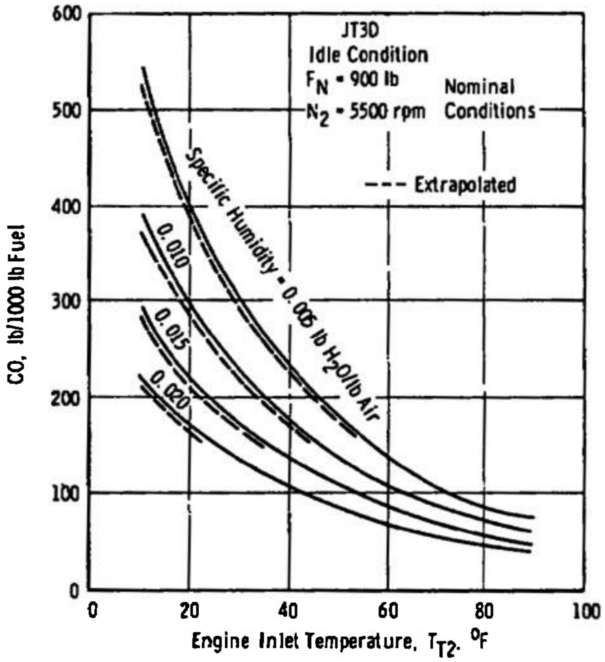


Fig. 2 Nitric Oxide Emission Data Correlation Corrected to 0.01 Humidity

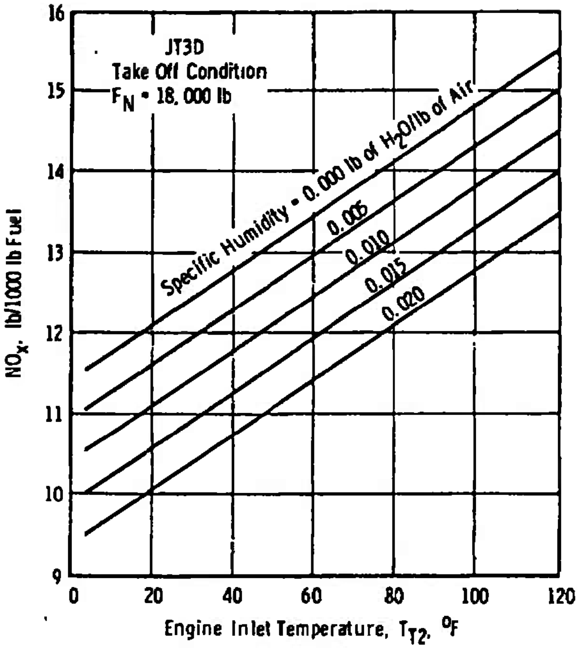


a. JT3D Environmental Test—Oxides of Nitrogen versus Burner Inlet Temperature (Corrected Data, High Power)

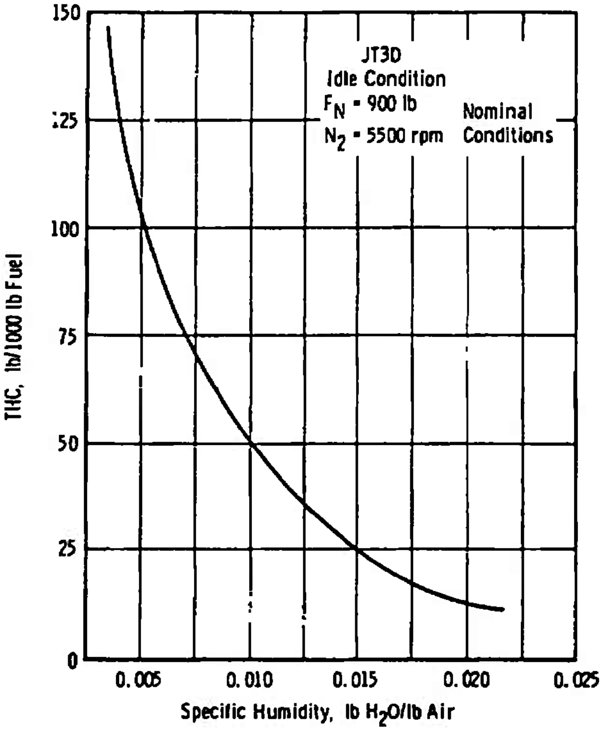


b. Correction Factor Curves for CO

Fig. 3 JT3D Emission Data Corrected for Humidity



c. Correction Factor Curves for NO_x



d. Correction Factor Curve for THC

Fig. 3 Concluded

TABLE I
EMPIRICAL FORMULAS FOR EMISSION LEVELS

Oxides of Nitrogen

$$EI_{NO_x} = 0.481 + 0.828 \times 10^{-3} F_N - 0.3655 \times 10^{-7} F_N^2 + 0.1513 \times 10^{-11} F_N^3 + 0.0337 T_{t2} - 101.18 \text{ SP HMD}$$

Carbon Monoxide

$$(1/EI_{CO})^{1/5} = 0.2148 + 0.355 \times 10^{-4} F_N + 0.177 \times 10^{-2} T_{t2} + 3.797 \text{ SP HMD}$$

Total Hydrocarbons

$$(1/EI_{THC})^{1/10} = 0.5481 + 0.360 \times 10^{-4} F_N + 9.699 \text{ SP HMD}$$

Where EI = Emissions Index, lb/1000 lb Fuel
F_N = Engine Thrust, lb
T_{t2} = Ambient (Inlet) Temperature, °F
SP HMD = Specific Humidity, lb H_2O/lb Air

The models were also used to develop correction factor curves for humidity and temperature changes where appropriate. These are shown in Figs. 1, and 3a through d.

(High Pressure Engines)

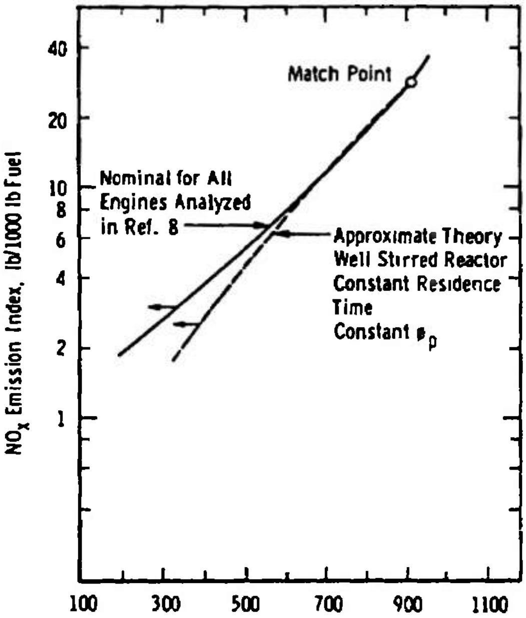


Fig. 4 Composite Nitric Oxide Emission Index

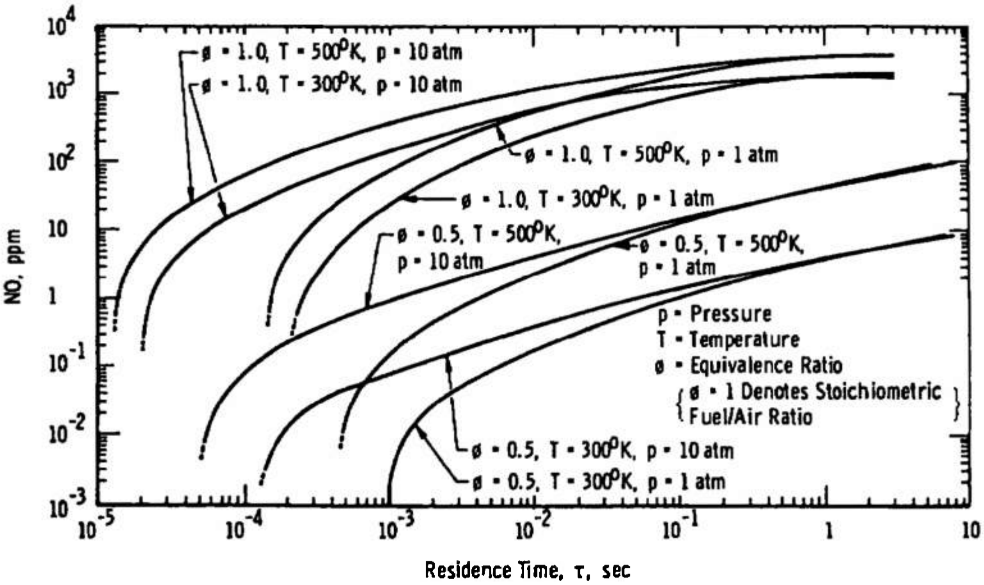


Fig. 5 Concentration of Nitric Oxide as a Function of Residence Time for Various Temperatures and Pressures—Adiabatic Reactor

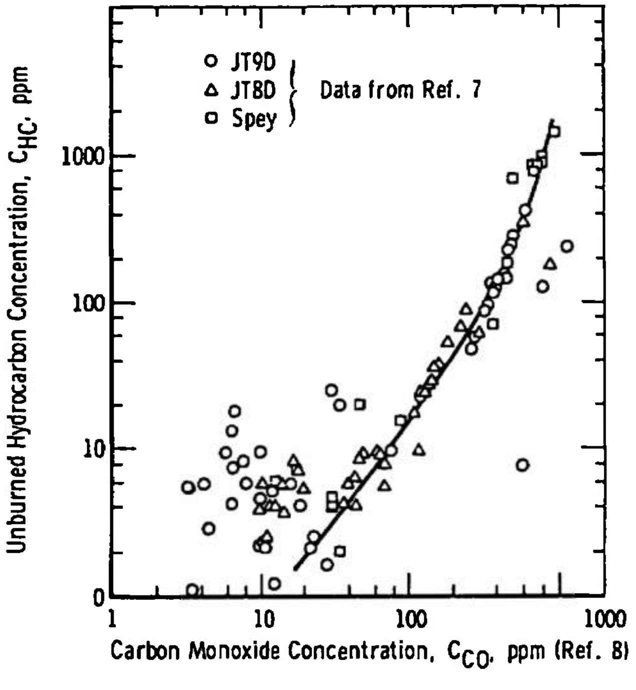


Fig. 6 Hydrocarbon/Carbon Monoxide Emission Correlation

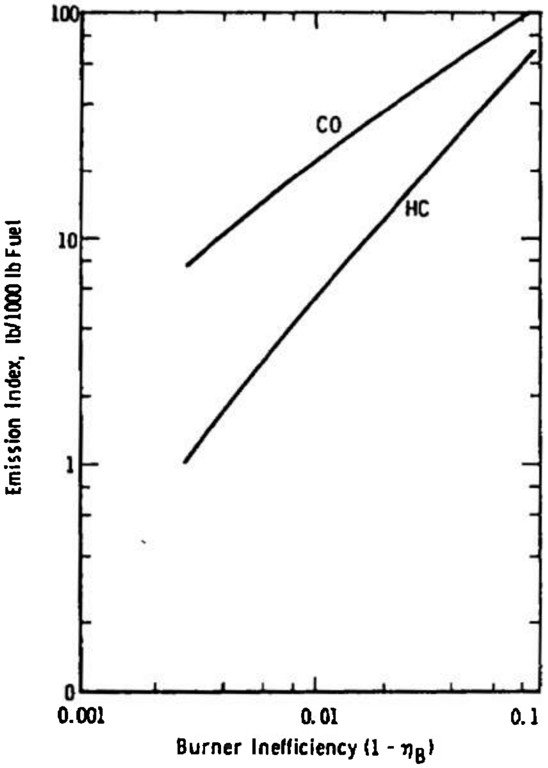


Fig. 7 Prediction of Carbon Monoxide and Hydrocarbon Emission Levels from Burner Efficiency

The importance of a good theoretical model which can account for the nonlinear response of combustor processes to changes in design and operating conditions is emphasized in the following example: "Smokeless" combustors were designed primarily by promoting better fuel/air mixing (injecting primary zone air into the fuel sprays and improving the distribution of liner cooling air to minimize hot spots, etc.). This reduced fuel rich regions; however, the higher average flame temperature expected was assumed to increase NO_x production. Lipfert (Ref. 8) showed that when sufficient data were statistically averaged, the expected increase was not apparent. It will be shown later that there is an almost complete inability to predict NO_x levels under fuel rich conditions; the observed effects of humidity are also not predictable. Thus. it can be concluded that current models are a poor representation of the details of most features of turbine combustor operation.

The following sections outline some of the research that has been conducted and attempts to define what combination of different approaches might lead to more quantitative accuracy in predicting pollutant emission levels and turbine combustor performance over the range of throttle settings. It is suggested that a model which predicts observed trends over the whole performance range is the most urgent task to be solved before realistic design changes may be recommended (to modify pollutant emission levels) to the machine shop.

SECTION II
EXISTING ANALYTICAL MODELS

The primary problem in modelling any practical combustion system is to account for turbulent mixing and chemical reaction simultaneously. Although mixing models have received intense interest over the years (Harsha, Ref. 13), it is only recently that an adequate representation of several classes of mixing flows (without combustion) could be obtained from one theory (Refs. 14 through 18). However, notable as these successes are, the theory is only applicable to simple flows involving two dimensions (planar or axial symmetry). Recently, progress has been made in techniques for including finite rate chemistry in a turbulent combustion model (again, a simple flow configuration) in which the time-average density in a nonhomogeneous reacting flow is obtained through an averaging model rather than as a function of the time-average pressure, temperature, and species concentration (Rhodes and Harsha, Ref. 19).

Combustors involve three-dimensional recirculating flows. Currently, no analytical model is capable of accurately representing such three-dimensional flows with recirculation. A technique for two-dimensional flows developed by Gosman, Ref. 20, is being actively developed by many research groups but is several years away from being a design tool for other than simple flows.

Currently, combustors are modelled by three groups of theories. The first group is based on calculating an augmented laminar flame speed (turbulent flame speed) as a function of the turbulence parameters of the flow. The chemical reaction rate is introduced by the use of this augmented laminar flame speed in laminar flame theory. The second group develops a microvolume burning concept by identifying eddies of size and lifetime dependent on the turbulence parameters. These eddies are assumed to burn either from the surface at the laminar flame speed or homogeneously throughout the volume. The third group of models assumes that the turbulence level is so high that the mixing time can be either neglected or is very small compared to the chemical reaction time (perfectly stirred reactor models). The combustion system is usually modelled as a combination of stirred reactor volumes. In a recent analysis (Ref. 21) the mixing rate is considered to be fast but finite compared to the chemical reaction rate (well-stirred reactors) and, in addition, includes plug flow in the primary zone to preserve the known hysteresis characteristics associated with blowout and relight.

2.1 TURBULENT FLAME SPEED MODELS

Turbulent flame speed models, developed primarily in Russia (Refs. 22 and 23) account for the effect of turbulence by calculating a turbulent flame speed based on analogy with the laminar flame speed (Refs. 24 and 25). This turbulent flame speed is then employed to calculate flame propagation from various ignition sources for determining required overall combustor dimensions and performance. The analysis has been developed for ramjet-type combustors of constant cross-sectional area with premixed combustibles and, hence, is not strictly applicable to turbine combustors.

In the highly turbulent combustor situation, burning is postulated to occur in a discrete zone. The forward boundary of this zone corresponds to ignition and is called the "flame front." The aft boundary of the zone is marked by the cessation of heat release; therefore, the zone thickness is determined by the chemical reaction rate (implying streamline flow through the zone) and gas transport properties. Combustor design is based on determining the size of the zone and its extent relative to the flameholder. The major deficiencies of this model, according to Hammond (Ref. 26). are the assumptions of smooth, premixed flames instead of the more realistic, highly irregular turbulent flames in which mixing plays a significant role as in practical turbine combustors. In addition, the turbulent flame speed has not been established as a proper characterization of the combustion process, and the exact dependence of the turbulent flame speed on reactant properties and combustor flow conditions has not been established.

2.2 MICROBURNING MODELS

The microvolume burning concept was introduced by Shchetinkov (Ref. 27) and represents an attempt to model both turbulent mixing and burning simultaneously.

Shchetinkov postulated mixing to be characterized by the formation and dissipation of turbulent eddies. These eddies are reasonably discrete masses of fluid which move as a particle relative to other eddies. Eddies containing burned or partially burned gases are carried out of the combustion zone by turbulent fluctuations, after which they mix with eddies of fresh gases. If the resulting eddies possess a sufficiently high temperature, ignition will occur and the eddy will burn. Shchetinkov modelled the mixing behavior by means of a grid of microvolume cubes of side 2ℓ where ℓ is the mixing length. The lifetime of the eddies was defined as $t = \ell/u$ where u is the turbulent intensity. The time available for combustion is

$$t_c = t - t_m - t_i$$

where t_m is a measure of the mixing rate within the eddy and t_i is an ignition delay time. Within the eddy. diffusion processes operate to equalize chemical composition and temperature; however, homogeneity is not always assured and both surface and volume combustion can occur. Shchetinkov considered only volume combustion (homogeneous) while Berl, et al. (Ref. 28) treated both.

This type of theory approximates the physical system rather closely, since in turbulent flow, eddies are formed which travel a certain mixing length and decay. However, uniformly sized eddies rather than a statistical size distribution is a poor assumption and theories for calculating mixing lengths are poorly developed. A more promising approach to the details of combustion in turbulence is that of Rhodes and Harsha (Ref. 19). They consider eddy classes to be formed with each eddy class corresponding to a prescribed concentration and a probability of existence at each point in the flow. The probability distribution functional form is assumed to be known; thus the mean and standard deviation define the value of the function. Assuming a Crocco relation between concentration and velocity, similar to that between velocity and enthalpy, the standard deviation is defined in terms of the axial velocity fluctuation which is related to the turbulent kinetic energy. Chemical reaction is incorporated by considering concentration classes as transient, perfectly stirred reactors (TPSR). A TPSR is one in which the feed rate and feed concentration may vary with time, and the time scale considered is short compared to the time required for the reactor to reach a steady-state condition. However, much more work is required to make this a viable theory for flows other than the simple axisymmetric flow considered in Ref. 19.

2.3 STIRRED REACTOR MODELS

A perfectly stirred reactor (PSR) is a region containing a homogeneous reacting mixture; therefore, if samples were taken from arbitrary locations in the zone, they would be identical in temperature, pressure, and chemical composition. The feed material is instantaneously mixed throughout the volume, thus maintaining the uniform composition of the zone, and an equal mass flow of exhaust products leaves the zone having the same composition as the reactor contents. The performance of the combustor is determined solely by chemical kinetics and, in general, the reactions do not progress to completion in the reactor.

The PSR concept was first applied to combustor modelling by Longwell and Weiss (Ref. 29). Initial attempts were based on an assumed single PSR for the combustor (Refs. 30 through 35). However, in a practical combustor (discussed later), the physical phenomena of blowout, a residual flame, hysteresis between blowout and relight, flame instability, incomplete mixing, etc., require more sophisticated models. Qualitative predictions of some of these phenomena were obtained by several authors (Refs. 34 through 38), primarily with the inclusion of recirculation of reaction products to one or more stirred reactors. The inclusion of detailed finite rate chemistry to a single PSR by Spalding Ref. 39, Jones (Ref. 40); and Jenkins (Ref. 41) provided the basis for the prediction of pollutants from turbine engines. Hammond and Mellor (Ref. 26) presented results of calculations assuming the turbine combustor could be modelled by a primary combustor (Fig. 8) consisting of two PSR's in parallel, i.e., a second reactor recycles part of the output of the first reactor; a secondary combustor, consisting of a series of plug-flow reactors (PFR) each fed with secondary air instantaneously mixed with the output of the previous reactor, followed by a final PFR fed with dilution air. As usual, the reactor volumes and recirculation rates were chosen arbitrarily. The injected fuel is all delivered to the first reactor with burnout achieved in

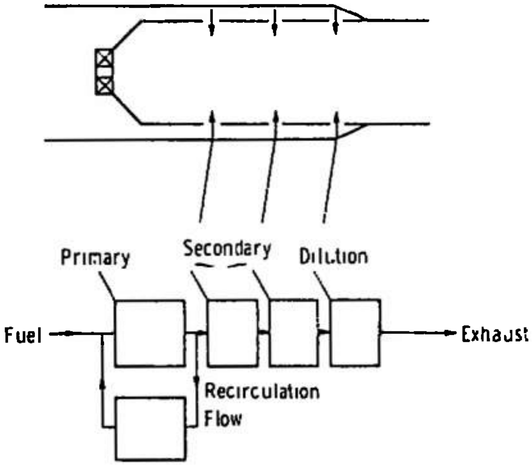


Fig. 8 Hammond's Recirculation Reactor Model

the PFR's in the secondary combustor. The model was modified by assuming part of the fuel was delivered to the second reactor (Ref. 42). Neither model is capable of predicting a characteristic delay time obtained when a recirculating PFR is included in the model, observed by Beer and Lee (Ref. 43) and shown to be essential for predicting flame stabilization phenomena (Refs. 26, 37, 21, and 44). This delay time is observed in transient flow tests in which a trace gas in the feed is suddenly cut off. Thus in a plug-flow recirculating model, tracer material is continuously recycled back through the stirred reactors. A trace gas monitor shows a characteristic delay time before tracer gas concentration follows the 1/e decay of stirred reactors.

The work reported by Swithenbank and co-workers (Refs. 21 and 44) represents the most complete analysis to date, with the exception of inability to calculate pollutant concentration. Their model is a development of the basic theory of Vulis (Ref. 35) and Swithenbank (Ref. 45) in which the primary combustor is modelled by two well-stirred reactors (WSR) in series. The well-stirred reactor is one in which the fuel and oxidant are mixed rapidly but not instantaneously. The two WSR's are coupled by a PFR which recirculates part of the second stirred reactor to the feed stream of the first (Fig. 9). The stirred reactors are modelled as well-stirred reactors by incorporating a mixing delay time. The mixing time is obtained from considerations of the turbulence level generated by total pressure losses in the air and fuel injection processes. In addition, entrainment theory is used to determine estimates of the individual reactor volumes and mass flows. More fundamental well-stirred reactor theories have previously been developed (Refs. 46 through 52), but none of these have been incorporated into more than a single reactor. They may be a logical extension of the Swithenbank model with the latter used for predicting the turbulence level, reactor volumes, mass flows, and hence residence times in a complex combustor such as in the turbojet. This model is readily extended to include

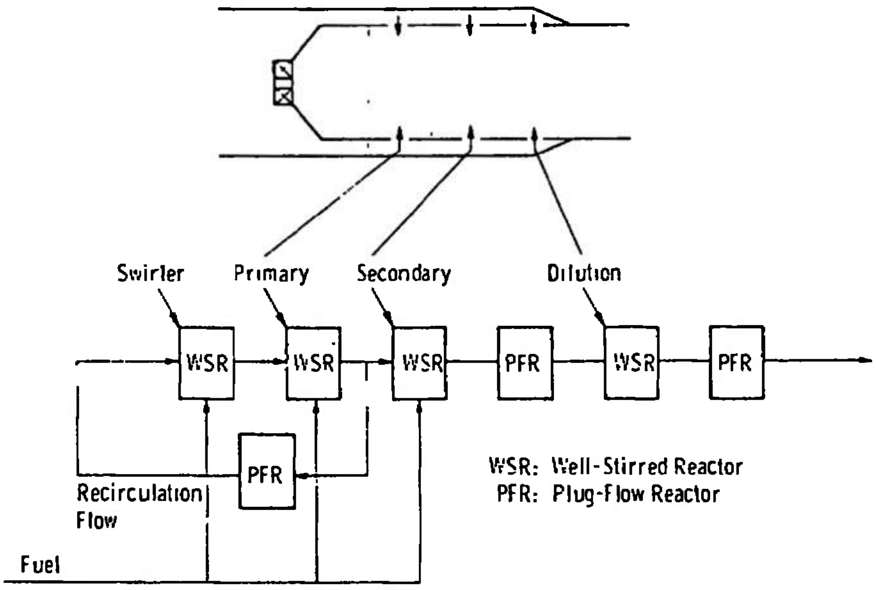


Fig. 9 Swithenbank's Recirculation Reactor Model

$aC_3H_8\ b(O_2 + N_2) \to c(\ \ )\ d(H_2O)\ (N_2)$

detailed pollutant concentrations since the necessary data, reactor volumes, and volume flow rates (hence reactor residence times) are determined. The utility of this model is considered sufficiently promising that details of the calculation of reactor volumes, flow rates, and some experimental evidence to substantiate the physical model are included. The ability to calculate individual reactor residence time is unique to this model, and the importance of this variable is shown in Fig. 5.

2.4 SWITHENBANK MODEL

The Swithenbank model is the result of several years of experience in modelling practical combustors and is oriented at a specific model of a turbojet-type combustor.

The experimental combustor, used by Swithenbank, is shown in Fig. 10, and the reactor volumes are shown schematically in Fig. 11. Rather than arbitrarily choosing the reactor volumes as did Hammond (Ref. 42), the method of Swithenbank is outlined to illustrate how they may be calculated.

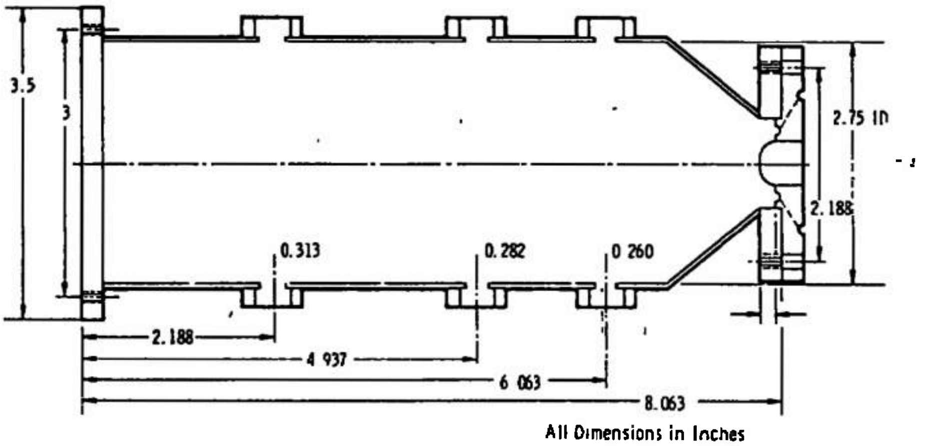


Fig. 10 Combustion Can

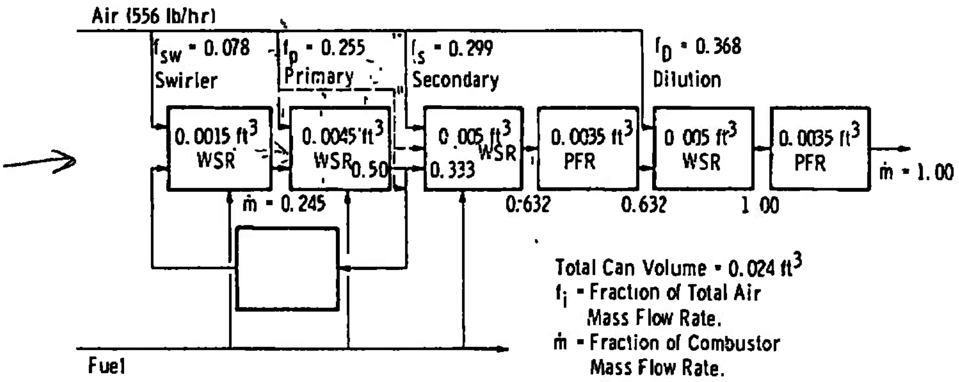


Fig. 11 Lycoming 2.75-in. Can: Proposed Interconnection of Reactors

2.4.1 Primary Zone

The primary combustor is modelled as a pair of stirred reactors coupled by a plug-flow reactor. The volumes and mass flows of the reactors are calculated using jet entrainment theory. The total primary zone volume is obtained by experiment or by inspection of the actual combustor being investigated. Swithenbank used a salt-tipped probe to determine the position on the combustor axis at which the whole flow field (primary zone) became sodium colored. If this procedure is not possible, the midpoint between the primary and secondary air inlet holes may be chosen. Although the swirler contributes to the primary flow, the primary air holes are largely responsible for the formation and intensity of the recirculation. The amount of recirculation can be predicted quite simply as follows:

The amount of flow entrained into a jet is given by (Ref. 53)

$$\frac{\dot{m}}{\dot{m}_j} = 0.32 \frac{x}{d_j} \sqrt{\frac{\rho}{\rho_j}}$$

$$d_j = d_o C_D$$

where $\dot{m}_j$ is the mass flow of air in the jet entering via an orifice of diameter d_o and discharge coefficient C_D, ρ_j is the air density, and x is the distance penetrated by the jet into the combustor. The distance available to entrain flow is the radius of the can.

Swithenbank assumed $\rho_j/\rho = 4$; however, ρ could readily be calculated assuming equilibrium combustion of 90 percent of the fuel in the primary zone. From Fig. 10, $x = 1.375$ in., $d_o = 0.26$ in., and C_D is given as 0.85; thus

$$\frac{\dot{m}}{\dot{m}_j} = 0.92$$

The primary region, therefore, behaves as a stirred reactor with 92 percent of the primary air mass flow entrained. Only a fraction (7.8/25.5 = 0.3) of this required entrainment mass flow is available from the swirler; thus 62 percent of the primary flow must be recycled into the swirler region. Measurements and water models of this type of flow have shown it to be relatively smooth flow; hence, it is treated as a plug-flow reactor. Addition of recycle flow to swirler flow takes place in the ratio 0.62/0.3 = 2.06. The strong shearing region in the swirler flow is treated as a stirred reactor.

The volumes of the individual reactors is estimated, assuming the gas density is the same in all the reactors: primary, recycle, and swirler. The volumes of the swirler and recirculation reactors are ratioed according to the mass flows in the reactors and that of the primary assuming it is symmetrical about the primary orifices.

2.4.2 Secondary and Dilution Zones

The secondary stirred reactor is also assumed to be symmetrical about the secondary orifice with its upstream boundary abutting the primary zone. The dilution zone stirred reactor is assumed to have the same volume for equal air mass flow. The secondary plug flow reactor lies between the secondary and dilution stirred reactors. There is no upstream recirculation in the secondary zone because there is more than sufficient mass flow to satisfy entrainment requirements:

$$\frac{\dot{m}}{m_j} = 0.32 \frac{x}{d_j} \sqrt{\frac{\rho}{\rho_j}}$$

Swithenbank assumes $\rho_j/\rho = 5$ in the secondary zone, giving $\dot{m}/m_j = 0.76$ i.e., the entrained flow is 76 percent of the secondary airflow. The mass flow upstream is $(25.5 + 7.8)/29.9 = 1.08$ times the secondary airflow and, hence, is more than sufficient to satisfy the entrainment appetite. The jet turbulence is assumed to dissipate rapidly (within a duct diameter) because of impingement of radially opposed jets; thus, little additional mixing should occur downstream of the secondary stirred reactor and the flow is assumed to be plug flow. The incomplete mass flow entrainment should result in a dip in the temperature profile at the axis. The dilution zone air entrains about 77 percent ($\rho_j/\rho = 4$) with 1.72 times the dilution air mass flow upstream. A significant dip in the temperature profile should be observed. Temperature measurements by Swithenbank confirmed this cold core as shown in Fig. 12.

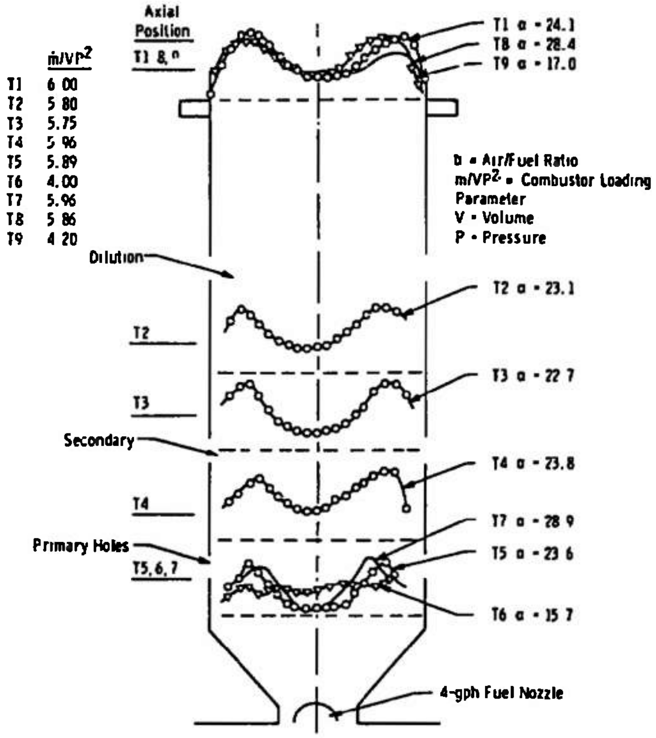


Fig. 12 Temperature Traverses

2.4.3 Fully Mixed Calculations

The mass flows, volumes, and residence times (volume/volume flow rate) having been determined, complete chemical kinetic calculations can be made. Additional input data required are inlet pressures and temperatures. The calculation can be initiated assuming equilibrium stoichiometric products from the second stirred reactor and plug-flow reactor in the primary zone are mixed with fuel and air from the swirler as feed to the first. The output calculated for the first reactor is fed to the second reactor together with the primary airflow. Part of the flow output is then recycled through a plug-flow calculation. The whole process is repeated until no further composition changes occur in each reactor. Calculations are then resumed for the secondary and dilution zone reactors. A comprehensive set of reactions and reaction rates is given in Table II.

TABLE II
CHEMICAL REACTIONS IN THE C/H/N/O SYSTEM

	Reaction	Reaction Rate			Ref.
		A	n	E	
1	$H + CO_2 = CO + OH$	5.6×10^{13}	0	23,500	106
2	$O + N_2 = NO + N$	1.44×10^{14}	0	75,580	107
3	$O + NO = N + O_2$	4.1×10^{9}	1	38,340	107
4	$N + OH = NO + H$	4.21×10^{13}	0	0	108
5	$OH + H_2 = H_2O + H$	2.2×10^{13}	0	5,150	106
6	$OH + OH = O + H_2O$	5.75×10^{12}	0	780	106
7	$O + H_2 = H + OH$	1.74×10^{13}	0	9,450	106
8	$H + O_2 = O + OH$	1.56×10^{14}	0	16,633	109
9	$O + H + M = OH + M$	3.6×10^{17}	-1	0	110
10	$O + O + M = O_2 + M$	3.6×10^{17}	-1	0	109
11	$H + H + M = H_2 + M$	1.81×10^{18}	-1	0	109
12	$H + OH + M = H_2O + M$	7.3×10^{18}	-1		109
13	$O + CO_2 = CO + O_2$	1.9×10^{13}	0	54,150	106
14	$CO + O + M = CO_2 + M$	6.0×10^{17}	-1	2,484	110
15	$N_2 + O_2 = N + NO_2$	2.7×10^{14}	-1	120,428	56
16	$N_2 + O_2 = NO + NO$	4.2×10^{14}	0	119,100	106
17	$NO + NO = N + NO_2$	3.0×10^{11}	0	0	106
18	$NO + M = O + N + M$	2.27×10^{17}	-0.5	148,846	56
19	$O + NO + M = NO_2 + M$	1.05×10^{15}	0	-1,870	105
20	$N + O_2 + M = NO_2 + M$	7.0×10^{11}	-1		56
21	$O + NO_2 = NO + O_2$	1.0×10^{13}	0	600	106
22	$H + NO_2 = NO + OH$	7.25×10^{14}	0	1,930	*
23	$N + CO_2 = CO + NO$	2.0×10^{11}	-0.5	7,950	*
24	$CO + NO_2 = NO + CO_2$	2.0×10^{11}	-0.5	4,968	*
25	$H + N_2O = OH + N_2$	3.01×10^{13}	0	10,800	108
26	$O + N_2O = O_2 + N_2$	3.61×10^{13}	0	24,800	107
27	$N_2 + NO_2 = NO + N_2O$	1.41×10^{14}	0	83,000	107

Reaction Rate Constant $k = AT^n \exp(-E/RT)$
Reverse Reaction Rate Constant Obtained from k and the Equilibrium Constant
*Recommended by R. B. Edelman

TABLE II (Concluded)

	Reaction	Reaction Rate			Ref.
		A	n	E	
28	$NO + HO_2 = OH + NO_2$	6.0×10^{11}	0	0	106
29	$O + N_2 + M = N_2O + M$	6.3×10^{14}	0	56,800	107
30	$H + O_2 + M = HO_2 + M$	1.5×10^{15}	0	-1,000	106
31	$H + HO_2 = OH + OH$	2.5×10^{14}	0	1,900	106
32	$OH + HO_2 = H_2O + O_2$	1.2×10^{13}	0	1,000	106
33	$O + HO_2 = OH + O_2$	5.0×10^{13}	0	1,000	106
34	$H + HO_2 = H_2 + O_2$	2.5×10^{13}	0	700	106
35	$H + HO_2 = O + H_2O$	1.0×10^{13}	0	1,000	106
36	$H_2 + HO_2 = H + H_2O_2$	1.9×10^{13}	0	24,000	106
37	$H_2O_2 + M = 2OH + M$	7.1×10^{14}	0	-5,100	106
38	$CH_4 + M \rightarrow CH_3 + H + M$	1.5×10^{19}	0	99,960	72
39	$CH_4 + H = CH_3 + H_2$	5.1×10^{13}	0	12,900	109
40	$CH_4 + OH = CH_3 + H_2O$	2.85×10^{13}	0	4,968	72
41	$CH_4 + O = CH_3 + OH$	1.7×10^{13}	0	8,700	72
42	$CH_3 + O_2 = HCO + H_2O$	1.0×10^{11}	0	0	72
43	$HCO + OH = CO + H_2O$	3.0×10^{13}	0	0	111
44	$H + CO + M = HCO + M$	1.0×10^{17}	-1	0	111
45	$HO_2 + HO_2 = H_2O_2 + O_2$	6.5×10^{13}	0	0	106
46	$H_2O_2 + H = H_2O + OH$	3.18×10^{14}		9,000	106
47	$CH_2 + 1/2\, O_2 \rightarrow CO + H_2$+	$5.52 \times 10^{8}\, p^{-0.825}$	1	24,642	79
48	$H + NO + M = HNO + M$	4.8×10^{15}		0	112
49	$HNO + H + M = H_2NO + M$				
50	$HNO + HNO + M \rightarrow H_2O + N_2O + M$				
51	$R + NO + M \rightarrow RNO + M$				
52	$R + RNO + M \rightarrow R_2NO + M$				
53	$R + R_2NO + M \rightarrow R_2NOR + M$				
54	$H + HNO = H_2 + NO$	1.4×10^{11}	0.5		113
55	$H + HCO = H_2 + CO$	2.0×10^{13}	0	0	111

+Any C_nH_m hydrocarbon is given this rate, however, with n CO molecules and m/2 H_2 molecules produced at this rate.

2.5 INCOMPLETE MIXING CALCULATIONS

At this point it is not clear how to account for incomplete mixing. Both Heywood (Ref. 54) and Bowman (Ref. 52) have carried out calculations, but Bowman has indicated deficiencies in his method. Heywood has not carried out calculations with more than one reactor in the primary zone; thus it is not clear how more reactors would influence the results. The method of Rhodes (Ref. 19) requires some estimate of turbulence intensity and Swithenbank's (Ref. 43) pressure loss calculation would supply an estimate. The rate of decay of turbulence could be obtained by the method of Corrsin (Ref. 46) as a first approximation.

Results of calculations with the fully mixed model should be generated, followed by an attempt to include the above incomplete mixing approaches to individual reactor volumes. Comparison of these results and with experimental data should determine what, if any, improvement in prediction capability has been achieved.

SECTION III
POLLUTANT CHEMISTRY MODELS

Several practical mathematical techniques now exist for solving the nonlinear algebraic equations which describe stirred reactor combustion for complete chemical kinetic schemes (Refs. 52, 55, and 56). A large number of solutions of problems involving pollutant production have been published (Refs. 26, 52, and 56 through 71). The analyses are characterized by their diverse opinions on the chemical reactions considered sufficient to describe the combustion process. Some reactions have been included in all analyses, although some differences in reaction rate constants are evident. These reactions include:

CO Oxidation:

1 $CO + OH = H + CO_2$

NO Formation: (Zel'dovich mechanism)

2 $O + N_2 = NO + N$
3 $N + O_2 = NO + O$
4 $N + OH = NO + H$

H_2 Oxidation:

5 $OH + H_2 = H_2O + H$
6 $OH + OH = O + H_2O$
7 $O + H_2 = H + OH$

8 $H + O_2 = O + OH$
9 $O + H + M = OH + M$
10 $O + O + M = O_2 + M$
11 $H + H + M = H_2 + M$
12 $H + OH + M = H_2O + M$

Additional reactions which have been included in various analyses are:

13 $CO + O_2 = CO_2 + O$
14 $CO + O + M = CO_2 + M$
15 $N_2 + O_2 = N + NO_2$
16 $N_2 + O_2 = NO + NO$
17 $N + NO_2 = NO + NO$
18 $O + N + M = NO + M$
19 $O + NO + M = NO_2 + M$

20 $N + O_2 + M = NO_2 + M$
21 $NO + O_2 = O + NO_2$
22 $H + NO_2 = NO + OH$
23 $N + CO_2 = CO + NO$
24 $CO + NO_2 = NO + CO_2$

Additional reactions which have been considered but not included in published calculations are:

25 $H + N_2O = OH + N_2$
26 $O + N_2O = O_2 + N_2$
27 $N_2 + NO_2 = NO + N_2O$
28 $NO + HO_2 = OH + NO_2$
29 $O + N_2 + M = N_2O + M$
30 $H + O_2 + M = HO_2 + M$
31 $H + HO_2 = OH + OH$
32 $OH + HO_2 = H_2O + O_2$
33 $O + HO_2 = OH + O_2$
34 $H + HO_2 = H_2 + O_2$
35 $H + HO_2 = O + H_2O$
36 $H_2 + HO_2 = H + H_2O_2$
37 $H_2O_2 + M = OH + OH + M$

3.1 HYDROCARBON COMBUSTION

A number of hydrocarbons have been investigated from methane to JP4 and JP5 fuels. The mechanism for methane combustion has received the most attention because of its simplicity compared to the higher molecular weight hydrocarbons.

38 $CH_4 + M = CH_3 + H + M$
39 $CH_4 + H = CH_3 + H_2$
40 $CH_4 + OH = CH_3 + H_2O$
41 $CH_4 + O = CH_3 + OH$
42 $CH_3 + O_2 = HCO + H_2O$
43 $HCO + OH = CO + H_2O$
44 $HCO + M = H + CO + M$

This mechanism was suggested by Marteney (Ref. 72) together with reactions 1, 2, 3, 18, 5, 6, 7, and 8. The mechanism was expanded by Bowman (Ref. 52) to include reactions 9, 10, 11, 29, 26, 20, 21, and 4. Similar mechanisms have been proposed by D'Souza (Ref. 73) and Seery (Ref. 74) with D'Souza also including reactions 30, 37, and

$$45 \quad HO_2 + HO_2 = H_2O_2 + O_2$$

$$46 \quad H_2O_2 + H = H_2O + OH$$

Species HO_2 and H_2O_2 are considered important in low temperature, high pressure, lean flames (Refs. 75 through 78). A common point of agreement in Ref. 52 and Ref. 66 seems to be that a global hydrocarbon reaction (Ref. 79) is adequate to represent pyrolysis of hydrocarbons for heat release rate calculations:

$$47 \quad C_nH_m + n/2\ O_2 \rightarrow nCO + m/2\ H_2$$

Prediction of NO_x concentrations has been shown to be excellent for premixed or flat flames with hydrogen, carbon monoxide, methane, and propane fuels, using reactions 2 and 3 (Refs. 66, 72, 73, 74, 80, and 81). An important point in NO production is the apparent high conversion of fuel N (as pyridines, quinolines, pyrroles, indoles or carbazoles) as shown in Refs. 69 and 82. Stirred reactor experiments (with separate fuel injection) have shown disagreements of up to an order of magnitude (Figs. 13 and 14) between measured and calculated NO levels with methane (Ref. 52) and propane (Ref. 68). The experiments with methane also involved the effect of poor mixing. Excellent

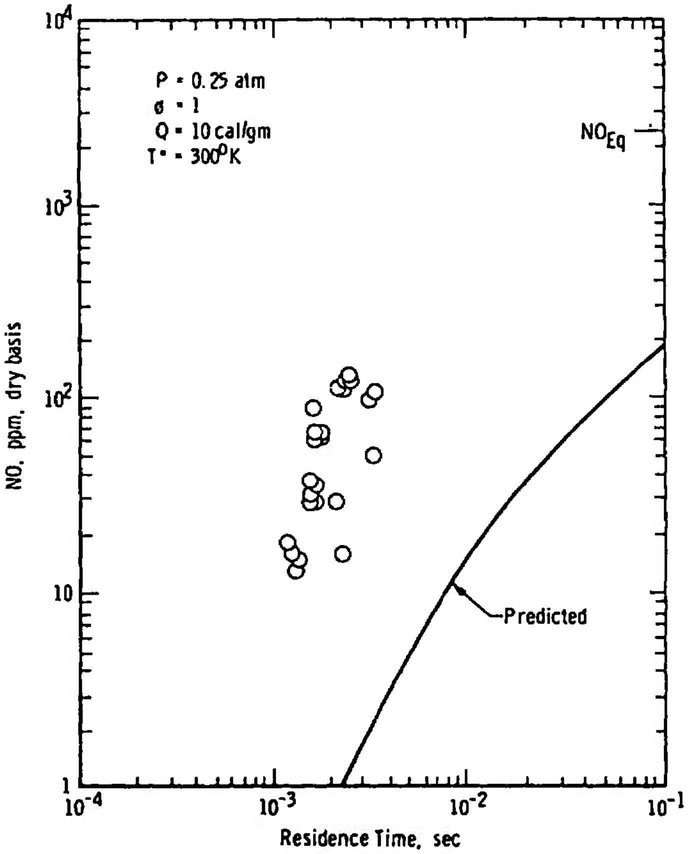


Fig. 13 Nitric Oxide as a Function of Residence Time

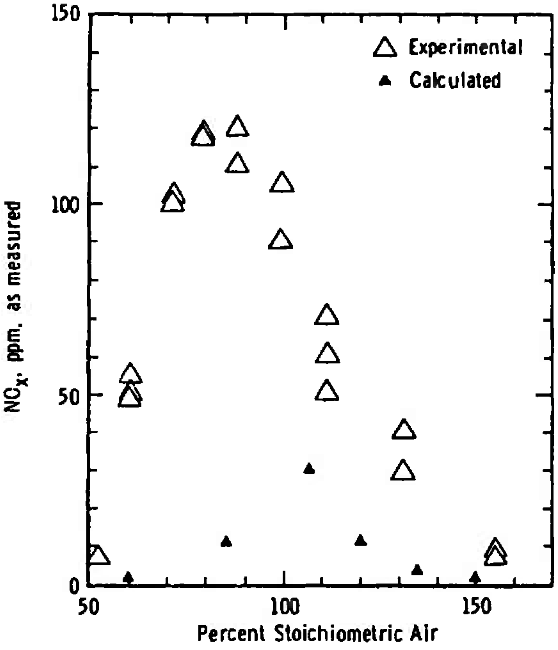


Fig. 14 Nitric Oxide as a Function of Percent Stoichiometric Air/Propane

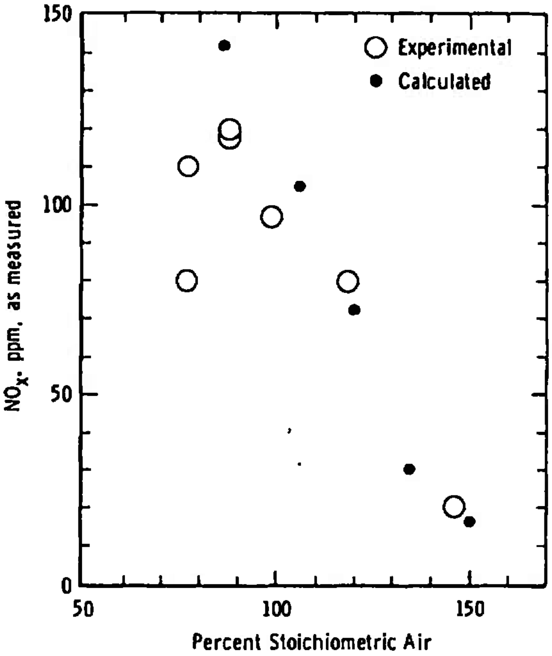


Fig. 15 Nitric Oxide as a Function of Percent Stoichiometric Air/Carbon Monoxide

agreement (Figs. 15 and 16) was obtained for carbon monoxide and hydrogen fuels (Ref. 68) and where the fuel and air were premixed (Ref. 41). If poor agreement is obtained in a controlled experiment such as with stirred reactors, it is not surprising that less than perfect agreement is obtained between engine emission data (Refs. 7, 11, 12, 58, 83, through 93) and predictions based on the single stirred reactor model of the primary combustor in Ref. 57 (data from Refs. 85, 91, and 92). The recent results obtained with the YJ-93 turbojet engine (Refs. 12 and 93), in which substantially different NO concentrations were measured by physically sampling according to SAE A.R.P. 1256 specification (Ref. 12) and in situ absorption spectroscopy (Ref. 93), are significant when comparing predictions with engine exhaust plane data. To date this difference has not been resolved. It is surprising that the

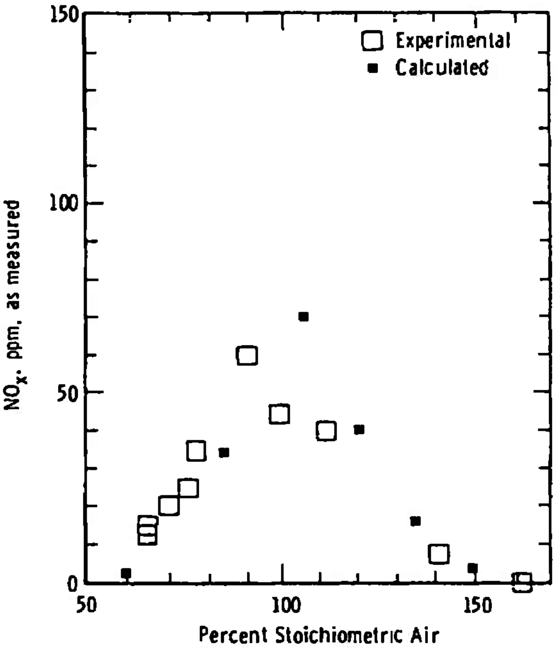


Fig. 16 Nitric Oxide as a Function of Percent Stoichiometric Air/Hydrogen

models of Ref. 54, 62, and 69 do as well as they do (less than an order of magnitude disagreement) since they assume equilibrium combustion of hydrocarbon and air in eddies, well mixed on a macroscale but not on a microscale, with assumed averaging techniques for NO production in the eddies. Equilibrium combustion ignores the "super-equilibrium" concentration of O atoms predicted by finite rate models, which can dominate the NO production (Ref. 72).

Reactions not considered previously may have a significance yet to be demonstrated. Hydrocarbons do not pyrolyze according to reaction 47, but rather through a complex chain of hydrocarbon fragments, each of which can react or pyrolyze further (Refs. 56 and 94). A possible fate of H atoms and hydrocarbon radicals (R) is:

48 $H + NO + M \rightarrow HNO + M$
49 $HNO + H \rightarrow H_2NO$
50 $M + HNO + HNO \rightarrow (HNO)_2 + M \rightarrow H_2O + N_2O + M$
51 $R + NO + M \rightarrow RNO + M$
52 $M + R + RNO \rightarrow R_2NO + M$
53 $R + R_2NO + M \rightarrow R_2NOR + M$

NO has long been employed as a scavenger of hydrocarbon radicals although usually at room temperatures (Ref. 95). This scavenging ability may have considerable importance in afterburners. The results of Ref. 12 indicate that NO virtually disappears on the centerline (total NO_x remained constant) of the General Electric (GE) YJ93 afterburner, where there was also a relatively high hydrocarbon concentration.

No concern has been given to the important effect (Refs. 96 and 97) of third body efficiencies in the above analyses. The majority of reactions are affected by the presence of other species either directly as in three-body reactions or indirectly through vibrational relaxation of species. H_2O and CO_2, for example, are efficient third bodies and, together with traces of alkali metals (always present as impurities), rapidly relax excited nitrogen molecules (Ref. 98). Reaction 14 is discussed in Ref. 99. Engelmann (Ref. 68) has shown that an important source of NO under fuel rich conditions is reaction 4, generating up to 20 percent of the total calculated value,

$$N + OH = H + NO$$

An alternate reaction may be considered (Ref. 96)

48 $H + NO + M \rightarrow HNO + M$

which is rapidly followed by (Ref. 100)

54 $H + HNO \rightarrow H_2 + NO$

or, if HNO >> H, reaction 50. Since the HNO is an excited state complex on formation, vibrational de-excitation of the molecule (eliminating the reverse of reaction 48 - dissociation) could play an important part in the net rate of reaction 54. A similar alternate reaction is (Ref. 96):

44 $H + CO + M \rightarrow HCO + M$
55 $H + HCO \rightarrow H_2 + CO$

Both these reactions and reaction 30 can remove H atoms (or hydrocarbon fragments) from the reaction chain with oxygen molecules and atoms and thus could alter the net rates of the nitrogen/oxygen reactions (more O atom available in reaction 2). Since some gas turbine combustors work at high pressures (up to 30 atm), these three-body reactions are favored.

3.2 SOOT AND SMOKE PRODUCTION

It is necessary to examine the process of fuel injection and evaporation in a turbine combustor to understand the mechanism for soot (smoke) production and consumption. The fuel is injected as a liquid cone via high pressure atomization nozzles producing sprays with typical droplet sizes ranging from 10 to 150 μ with Sauter mean diameters of about 70 μ. The cone, which may be solid or hollow, is generally swirled, and has an included angle between 60 and 80 deg. The formation of a stable spray from the liquid "sheet" occurs within a fuel nozzle diameter, and thus interaction with primary zone gases is usually between discrete droplets. The liquid drops evaporate at a finite rate (providing the combustor pressure is less than the critical pressure of the fuel); hence, following the models of Refs. 21, 65, and 101, part of the fuel remains liquid until it reaches the second reactor and recirculation flow, i.e., it traverses the first reactor intact. All models consider each reactor to be essentially stoichiometric (and thus generate high flame temperatures) but neglect the liquid fuel fraction implied in models including more than one reactor. Thus, if these models are correct, ideal conditions exist for thermal decomposition of fuel to soot and hydrocarbon fragments, both in the vicinity of the injector and in the first reactor. Since only about 90 percent of the fuel is burnt in the primary combustor and 9+ percent in the secondary (Ref. 102), some of the fuel goes right through to the turbine and exhaust. The effects of engine operating variables such as pressure, temperature, mass flow rates, etc., on fuel droplets and drop lifetimes/residence times is discussed in detail in Refs. 101 and 103. The principal conclusion of Ref. 103 concerning smoke production is that soot and smoke are primarily a result of inadequate mixing.

Expressions for soot and smoke production rates are not available in terms of detailed reactions and rates. It is possible to estimate these using experimental engine data, if the correlations of Refs. 8 and 9 are accepted. Thus if a relationship could be found which relates soot particulates (measured as a smoke number) to the hydrocarbons, C_xH_y (measured as equivalent methane, CH_4) and the relationship between CO and C_xH_y of Refs. 8 or 9 is used, then an approximate method of accounting for fuel fragments and their subsequent chemistry downstream of the primary zone is available. Of course, no information is furnished on hydrocarbon fragment chemistry in the primary zone. A different correlation is required for different engines as discussed previously.

Expressions for soot consumption have been determined (Refs. 104 and 105). Soot consumption was correlated by the partial pressure of hydroxyl radicals in Ref. 105. Heywood (Ref. 61) showed that the data of Ref. 105 were taken over a broader range of oxygen pressures but that neither were in the range of turbine operating conditions. This is an area in which research is necessary before reactions and rates can be prescribed to properly account (quantitatively) for soot and smoke production and consumption.

SECTION IV
DISCUSSION

The preceding sections outline the current state-of-the-art in turbojet combustor modelling. Models which comprise a series of reactors which include combinations of stirred reactors linked with plug-flow zones are recommended because they alone are capable of predicting gross operating characteristics correctly. A method of estimating the individual reactor volumes, volume flow rates, and particle residence times is suggested using jet entrainment theory. Unfortunately, no recommendations are established for successful emission predictions, although the list of chemical reactions is long. The major problem lies in the absence of detailed calculations which assess the importance of (1) including finite rate fuel evaporation to a global hydrocarbon combustion' model, (2) including reactions between hydrocarbon (fragments) and nitric oxide, and (3) ignoring both the relative cool regions where liner cooling air is admitted and the core flow which is not entrained by the secondary and dilution air jets. In addition to these problems, consideration must also be given to the fact that both temporal and spatial inhomogenieties exist - as witnessed by the soot and smoke emission from engines. Methods have been developed to predict the effects of incomplete mixing; however, no multiple reactor calculations have been carried out with any of these methods, and inadequacies have been reported for single reactor calculations. An alternate approach is outlined; however, significant development work will be required before it can be evaluated. Finally, it seems that no scheme is available for detailing the process by which hydrocarbons are thermally degraded to reacting species, soot and smoke. It is evident that much research needs to be done before accurate models of turbojet combustor (and afterburner) processes are developed. The author firmly believes that a major fault of most models outlined previously is the inability to predict operating characteristics such as combustor hysteresis, particle residence times, and the effects of incomplete mixing. It is suggested that the two former parameters should be attended to and substantial effort initiated to solve the latter problem.

SECTION V
CONCLUDING REMARKS

The turbojet combustor is a very complicated component, and quantitative calculations of performance characteristics and emission levels require a complex analytical model. The Swithenbank model will generate the right qualitative results and it remains to be seen if quantitative accuracy is achieved. Inclusion of incomplete mixing is essential if the range of throttle settings from idle to takeoff is to be included. Much work is necessary on soot and unburned hydrocarbon production rates; however, the method suggested in this report should provide a reasonable estimate. If the model (chemical and fluidynamics) is shown to be correct at any one throttle setting, then at least some confidence in the chemical model will have accrued. Without this confirmation, there will be no mutually satisfactory basis for determining whether spectroscopic or physical gas analysis gives the right results when substantial differences are observed (as reported in Refs. 12 and 93). These differences are important and should be resolved since they may incorrectly bias the results of Environmental Impact Statements and the Climatic Impactment Assessment Program.

REFERENCES

1. Gradon, K. and Miller, S.C. "Combustion Development on the Rolls-Royce Spey Engine." Combustion in Advanced Gas Turbines, Ed. I.E. Smith, Pergamon Press, 1967, p. 45.

2. Toone, B. "A Review of Aero Engine Smoke Emission." Combustion in Advanced Gas Turbines. Ed. I.E. Smith, Pergamon Press, 1967, p. 271.

3. Niki, H. "Mechanism of Smog Reactions." Ford Motor Company Scientific Research Staff, April 1972.

4. Leighton, P.A. Photochemistry of Air Pollution. Academic Press, New York, 1961.

5. Wayne, L.G. "On the Mechanism of Photo-Oxidation in Smog." Archives of Environmental Health, Vol. 7, 1963, p. 229.

6. Jackson, S.R. and Odgers. J. "Factors Affecting Heat Release in Combustion Chambers and Consideration of the Related Materials and Structures." Combustion in Advanced Gas Turbines, Ed. I.E. Smith, Pergamon Press, 1967, p. 173.

7. Bogdan, L. and McAdams, H.T. "Analysis of Aircraft Exhaust Emissions Measurements." CAL-NA-5007-K-1 Cornell Aeronautical Laboratories, 1971.

8. Lipfert, F.W. "Correlation of Gas Turbine Emission Data." ASME Paper 72-GT-60, 1972.

9. Nelson, A.W., Davis, J.C., and Medlin, C.H. "Progress in Techniques for Measurement of Gas Turbine Engine Exhaust Emissions." AIAA Paper No. 72-1199, AIAA-SAE Joint Propulsion Specialists Conference, Nov. 1972.

10. Edelman, R. and Weilerstein, G. "A Theoretical Study of Combustion and NO Formation in Well Mixed Regions." GASL-TR-758, General Applied Science Laboratories, Inc., 1971.

11. Lazalier, G.R. and Gearheart, J.W. "Measurement of Pollutant Emissions from an Afterburning Turbojet Engine at Ground Level: I. Particulate Emissions." AEDC-TR-72-64 (AD744048), 1972, and "II. Gaseous Emissions," AEDC-TR-72-70 (AD747773), Aug. 1972.

12. Neely, J. and Davidson, D.L. "Emission Level of the YJ93-GE-3 Engine, an SST-Like Engine." 2nd Conference on Climatic Impact Assessment Program, Cambridge, Mass., 1972.

13. Harsha, P.T. "Free Turbulent Mixing: A Critical Evaluation of Theory and Experiment." PhD. Dissertation, University of Tennessee, 1970; also AEDC-TR-71-36 (AD718956), Feb. 1971.

14. Harsha, P.T. "Prediction of Free Turbulent Mixing Using a Turbulent Kinetic Energy Method." Presented at Langley Working Conference on Free Turbulent Shear Flows, NASA Langley Research Center, July 1972, NASA SP in preparation.

15. Peters, C.E. and Phares, W.J. "An Integral Turbulent Kinetic Energy Analysis of Free Shear Flows." Presented at Langley Working Conference on Free Turbulent Shear Flows, NASA Langley Research Center, July 1972, NASA SP in preparation.

16. Rudy. D.H. and Bushnell, D.M. "Use of Prandtl's Mixing Length Model in Free Turbulent Flow Calculations." Presented at Langley Working Conference on Free Turbulent Shear Flows. NASA Langley Research Center, July 1972, NASA SP in preparation.

17. Launder, B.E., Morse. A., Rode, W., and Spalding, D.B. "The Prediction of Free Shear Flows–A Comparison of the Performance of Six Turbulent Models." Presented at Langley Working Conference on Free Turbulent Shear Flows. NASA Langley Research Center, July 1972, NASA SP in preparation.

18. Smith. M.A. and Heck, P.M. "Turbulent Kinetic Energy Solutions for Compressible Free Turbulent Mixing." Presented at Langley Working Conference on Free Turbulent Shear Flows, NASA Langley Research Center, July 1972, NASA SP in preparation.

19. Rhodes. R.P. and Harsha. P.T. "On Putting the 'Turbulent' in Turbulent Reacting Flow." AIAA Paper No. 72-68, AIAA 10th Aerospace Sciences Meeting, San Diego, California, Jan. 1972.

20. Gosman, A.D. et al. Heat and Mass Transfer in Recirculating Flows. Academic Press, London, 1969.

21. Swithenbank, J., Poll, I., Wright, D.D., and Vincent, M.W. "Combustor Design Fundamentals." 14th Symposium (International) on Combustion, Penn. State University, Aug. 1972, to be published by The Combustion Institute.

22. Il'ashenko, S.M. and Talantov, A.V. "Theory and Analysis of Straight-Through-Flow Combustion Chambers." Izdatelistvo, "Machinostroyeniye", Moskva 1, 1964.

23. Talantov, A.V. "Analysis of Performance of the Simplest Ramjet Combustion Chamber Under Flight Conditions." Izvestia Vysshikh Uchebykh Zavedeniy, MOV SSSR, Seriya Aviatsionnaya Tekhnika 2, 1959, p..122.

24. Zel'dovich, Ya. B. Journal of Technical Physics (U.S.S.R.), 14, 1944, p. 3.

25. Williams, G.C., Hottel, H.C., ,and Scurlock, A.C. "Flame Stabilization and Propagation in High Velocity Gas Streams." 3rd Symposium on Combustion, Flame and Explosion Phenomena, Williams and Wilkins, 1949, p. 21.

26. Hammond, D.C., Jr. and Mellor, A.M. "A Preliminary Investigation of Gas Turbine Combustor Modelling." Comb. Sci. and Tech., 2, 1970, p..67.

27. Shchetinkov, E.S. "Calculation of Flame Propagation in a Turbulent Flow." Proceedings of the Moscow Seminar on Combustion, Energetics Institute, USSR Academy of Science, Izdatel'stvo, Adademia Nauk SSSR, Moskva 1, 1959.

28. Berl, V.G., Rice, J.L. and Rosen, P. "Flames in Turbulent Streams." Jet Propulsion. 25, 1955, pp. 341-346.

29. Longwell, J.P. and Weiss, M.A. "Flame Stability in Bluff Body Recirculation Zones." Ind. Eng. Chem., 45, 1953, pp. 1629-1633.

30. Longwell, J.P., Frost, E.E., and Weiss, M.A. "High Temperature Reaction Rates in Hydrocarbon Combustion." Ind. Eng. Chem., 47, 8, 1955, p. 1634.

31. Longwell, J.P. and Weiss, M.A. "Heat Release Rates in Hydrocarbon Combustion." IME-ASME Joint Conference on Combustion. M.I.T., published by the Institute of Mech. Eng., London, pp. 334-339.

32. Weiss, M.A., Lang, J.L., and Longwell, J.P. "Combustion Rates in Spherical Reactors." Ind. Eng. Chem., 50, 2, 1958, p. 247.

33. Egerton, A.C., Saunders, O.A. and Spalding, D.B. "The Chemistry and Physics of Combustion." IME-ASME Joint Conference on Combustion, M.I.T., Cambridge, Mass.. June 1955, published by the Institute of Mech. Eng., London, pp. 14-33.

34. Hottel, H.C., Williams, G.L., and Baker, M.L. "Combustion Studies in a Stirred Reactor." 6th Symposium (International) on Combustion, Aug. 1956, Reinhold, New York, 1957, p. 389.

35. Vulis, L.A. Thermal Regimes of Combustion. Meljran Hill, New York, 1961.

36. Spalding, D.B. "Theoretical Relationships between Combustion Intensity and Pressure Drop for One-Stream Combustion Chambers." ARC 19, 180, C.F. 393, Aeronautical Research Council, Apr. 1957.

37. Hottel, H.C., Williams, G.L., and Bonnell, A.H. "Application of Stirred Reactor Theory to the Prediction of Combustor Performance." Comb. and Flame, 2, p. 13, 1958.

38. Jain, V.K. and Spalding, D.B. "The Effects of Finite Recirculation in a Stirred Reactor." Comb. and Flame, 10, 1966, p. 37.

39. Spalding, D.B. "The Theory of Flame Phenomena with a Chain Reaction." Phil. Trans. Roy. Soc. (London), 249, A957, 1956, p. 1.

40. Jones, A. and Prothero, A. "The Solution of the Steady-State Equations for an Adiabatic Stirred Reactor." Comb. and Flame. 12, 5, 1968, p. 457.

41. Jenkins, D.R. and Yumlu. V.S. "Combustion of Hydrogen and Oxygen in a Steady Flow Adiabatic Stirred Reactor." 11th Symposium (International) on Combustion, The Combustion Institute, 1967, p. 779.

42. Hammond, D.C. and Mellor, H.M. "Analytical Calculations for the Performance and Pollutant Emissions of Gas Turbine Combustors." AIAA Paper No. 71-711, AIAA/SAE 7th Propulsion Joint Specialists Conference, Salt Lake City, June 1971.

43. Beer, J.M. and Lee, K.B. "The Effect of the Residence Time Distribution on the Performance and Efficiency of Combustors." 10th Symposium (International) on Combustion, The Combustion Institute, 1965, p. 1187.

44. Poll, I. "A Theoretical Analysis of Mixing and Recycle in Propane/Air Combustors." HIC 161, University of Sheffield, England, May 1971.

45. Swithenbank, J. "Combustion Fundamentals." USAF/OSR/70/2110TR (AD710321), Feb. 1970.

46. Corrsin, S. "Simple Theory of an Idealized Turbulent Mixer." A. I. Ch. E. J., 3, 3, 1957, p. 329.

47. Zwietering, T.N. "The Degree of Mixing in Continuous Flow Systems." Chem. Eng. Sci., 11, 1, 1959.

48. Curl, R.L. "Dispersed Phase Mixing· I. Theory and Effects in Simple Reactors." A. I. Ch. E. J., 9, 2, 1963, p. 175.

49. Ng, D. Y. C. and Rippin, D. W. T. "The Effect of Incomplete Mixing and Conversion in Homogeneous Reactions." 3rd Symposium (European) on Chemical Reaction Engineering, Amsterdam, Pergamon Press, Oxford, 1964, p. 161.

50. Evangelista, J. J., Katz, S., and Shinnar, R. "Scale-Up Criteria for Stirred Tank Reactors." A. I. Ch. E. J., 15, 6, 1969, p. 843.

51. Evangelista, J.J., Shinnar, R., and Katz, S. "The Effect of Imperfect Mixing on Stirred Combustion Reactors." 12th Symposium (International) on Combustion, The Combustion Institute, 1969, p. 901.

52. Bowman, B.R., Pratt, D.T., and Crowe, C.T. "Effects of Turbulent Mixing and Chemical Kinetics on Nitric Oxide Production in a Jet-Stirred Reactor." 14th Symposium (International) on Combustion, Penn. State University, Aug. 1972, to be published by The Combustion Institute.

53. Swithenbank, J. and Chigier, N. "Vortex Mixing for Supersonic Combustion." 12th Symposium (International) on Combustion, The Combustion Institute, 1969, p. 1153.

54. Heywood, J.B. "Gas Turbine Combustor Modelling for Calculating Nitric Oxide Emissions." AIAA Paper No. 71-712, AIAA Paper No. 71-713, AIAA/SAE 7th Propulsion Joint Specialists Conference, Salt Lake City, Utah, 1971.

55. Osgerby, I.T. "An Efficient Numerical Method for Stirred Reactor Calculations." AEDC-TR-72-164 (AD751462), and AFOSR-TR-72-0910, Nov. 1972.

56. Edelman, R. and Economos, C. "A Mathematical Model for Jet Engine Combustor Pollutant Emissions." AIAA Paper No. 71-714, AIAA/SAE 7th Propulsion Joint Specialists Conference, Salt Lake City, Utah, 1971.

57. Smith, D., Sawyer, R.F., and Starkman, E.S. "Oxides of Nitrogen from Gas Turbines." J. of the Air Pollution Control Assn. 18, 1968, p. 30.

58. Sawyer, R.F. and Starkman, E.S. "Gas Turbine Exhaust Emissions." SAE Paper No. 680 462, 1968.

59. Caretto, L.S., Sawyer, R.F., and Starkman, E.S. "The Formation of Nitric Oxide in Combustion Process." 1968 Technical Meeting, Central States Section, The Combustion Institute, 1968.

60. Starkman, E.S., Mizutani, Y., Sawyer, R.F., and Teixeira, D.P. "The Role of Chemistry in Gas Turbine Emissions." ASME Paper No. 70-GT-81, 1970.

61. Heywood, J.B., Fay, J.A., and Linden, L.H. "Jet Aircraft Air Pollutant Production and Dispersion." AIAA Paper No. 70-115, 8th Aerospace Sciences Meeting, 1970.

62. Fletcher, R.S. and Heywood, J.B. "A Model for Nitric Oxide Emissions from Aircraft Gas Turbine Engines." AIAA Paper No. 71-123, AIAA 9th Aerospace Sciences Meeting, New York, N.Y., Jan. 25027, 1971.

63. Pratt, D.T., Bowman, B.R., Crowe, C.T., and Sonnichsen, T.W. "Prediction of Nitric Oxide Formation in Turbojet Engines by PSR Analysis." AIAA Paper No. 71-713, AIAA/SAE 7th Propulsion Joint Specialists Conference, Salt Lake City, Utah, 1971.

64. Hammond, D.C. and Mellor, A.M. "Analytical Calculations for the Performance and Pollutant Emissions of Gas Turbine Combustors." AIAA Paper No. 71-711, AIAA Paper No. 71-713, AIAA/SAE 7th Propulsion Joint Specialists Conference, Salt Lake City, Utah, 1971.

65. Roberts, R., Aceto, L.D., Kollrack, R., Bonnell, J.M., and Teixeira, D.P. "An Analytical Model for Nitric Oxide Formation in a Gas Turbine Combustion Chamber." AIAA Paper No. 71-715, AIAA Paper No. 71-713, AIAA/SAE 7th Propulsion Joint Specialists Conference, Salt Lake City, Utah, 1971.

66. Carretto, L.S., Muzio, L.P., Sawyer, R.F., and Starkman, E.S. "The Role of Kinetics in Engine Emission of Nitric Oxide." Comb. Sci. and Tech., 3, 1971, p. 53.

67. Carretto, L.S. "Modelling Pollutant Formation in Combustion Processes." 14th Symposium (International) on Combusion, Penn. State University. 1972, to be published by The Combustion Institute.

68. Engelmann, V.S., Edelman, R.B., Bartok, W., and Longwell, J.P. "Experimental and Theoretical Studies of NO_x Formation in a Jet-Stirred Combustor." 14th Symposium (International) on Combustion, Penn. State University, 1972, to be published by The Combustion Institute.

69. Appleton, J.P. and Heywood, J.L. "The Effects of Imperfect Fuel-Air Mixing in a Burner on NO Formation from Nitrogen in the Air and Fuel." 14th Symposium (International) on Combustion, Penn. State University, 1972, to be published by The Combustion Institute.

70. Bowman, C.T. "Kinetics of Nitric Oxide Formation in Combustion Processes." 14th Symposium (International) on Combustion, Penn. State University, 1972, to be published by The Combustion Institute.

71. Newhall, H.K. "Kinetics of Engine Generated Nitrogen Oxides and Carbon Monoxide." 12th Symposium (International) on Combustion, The Combustion Institute, 1969.

72. Marteney, P.J. "Analytical Study of the Kinetics of Formation of Nitrogen Oxide in Hydrocarbon-Air Combustion." Comb. Sci. and Tech., 1, 1970, p. 461.

73. D'Souza, M.V. and Karim, G.A. "An Analytical Study of Methane Oxidation in a Steady-Flow Reactor." Comb. Sci. and Tech., 3, 1971, p. 83.

74. Seery, D.J. and Bowman, C.T. "An Experimental and Analytical Study of Methane Oxidation Behind Shock Waves." Comb. and Flame, 14, 1970, p. 37.

75. Fristrom, R.M. and Westenberg, A.A. Flame Structure. McGraw Hill, New York, 1965, p. 341.

76. Enckolopyan, N.S. "Kinetics and Mechanism of Methane Oxidation." 7th Symposium (International) on Combustion, Butterworths Scientific Publications, London, 1959, p. 157.

77. Blundell, R.V., Cook, W.G.A., Hoare, D.E., and Milne, G.S. "Rates of Radical Reactions in Methane Oxidation." 10th Symposium (International) on Combustion, The Combustion Institute, 1965, p. 445.

78. Getzinger, R.W. and Schott, G.L. "Kinetic Studies of OH Radicals in Shock Waves. V. Recombination via the $H + O_2 + M \rightarrow HO_2 + M$ Reaction in Lean Hydrogen-Oxygen Mixtures." J. Chem. Phys., 43, 9, 1965. p. 3237.

79. Edelman, R.B. and Fortune, O.F. "A Quasi-Global Chemical Kinetic Model for the Finite Rate Combustion of Hydro-Cargon Fuels with Application to Turbulent Burning and Mixing in Hypersonic Engines and Nozzles." AIAA Paper No. 69-86, AIAA 7th Aerospace Sciences Meeting, 1969.

80. Bowman, C.T. "Investigation of Nitric Oxide Formation Kinetics in Combustion Process: The Hydrogen-Oxygen-Nitrogen Reaction." Comb. Sci. and Tech., 3, 1971, p. 37.

81. Lindsey, J.B., Roberts. A.B., and Williams, A. "The Formation of Oxides of Nitrogen in Some Flames." Comb. Sci. and Tech. 4, 1971, p. 9.

82. Bracco, F.V. "Nitric Oxide Formation in Droplet Diffusion Flames." 14th Symposium (International) on Combustion, Penn. State University, 1972, to be published by The Combustion Institute.

83. Bastress, E.K. and Fletcher, R.S. "Nature and Control of Aircraft Engine Exhaust Emissions." NREC Report No. 1134-1, Northern Research and Engineering Corporation, Cambridge, Mass., 1968.

84. Sawyer, R.F., Teixera, D.P. and Starkman, E.S. "Air Pollution Characteristics of Gas Turbine Engines." Trans. ASME., J. Eng. Power, 10, 1969, p. 290.

85. Lozano, E.R., Melvin, W.W., and Hochheiser, S. "Air Pollution Emissions from Jet Engines." J. of the Air Pollution Control Assn., 18, 1968, p. 392.

86. Bahr, D.W. "Control and Reduction of Aircraft Turbine Engine Exhaust Emissions." Symposium on Emissions from Continuous Combustion Systems, G.M. Research Laboratories, 1971.

87. Nelson, A.W. "Exhaust Emissions Characteristics of Aircraft Gas Turbine Engines." ASME Paper 72-GT-75, Paper presented at the Gas Turbine and Fluids Engrg. Conf. and Prod. Show, March 26-30, 1972.

88. Hazard, H.R. "NO_x Emission from Experiment Compact Combustors." ASME Paper, 72-GT-108, Paper presented at the Gas Turbine and Fluids Engrg. Conf. and Prod. Show, March 26-30, 1972.

89. Grobman, J. "Effect of Operating Variables on Pollutant Emissions from Aircraft Turbine Engine Combustors." NASA TMX-67887, Sept. 1971.

90. Briehl, D.. Papathakos, L., and Strancar, R.J. "Effect of Operating Conditions on the Exhaust Emissions from a Gas Turbine Combustor." NASA TN D-6661, Feb. 1972.

91. George, R.E. and Burlin, R.M. "Air Pollution from Commercial Jet Aircraft in Los Angeles County." Los Angeles Air Pollution Control District, Los Angeles, California, Apr. 1960.

92. Smith, D., Sawyer, R.F., and Starkman, E.S. "Oxides of Nitrogen from Gas Turbines." SAE Preprint 680347, Apr. 1968.

93. McGregor, W.K., Seiber, B.L.. and Few. J.D. "Concentration of OH and NO in YJ93-GE-3 Engine Exhausts Measured in Situ by Narrow Line UV Absorption." 2nd Conference on Climatic Impact Assessment Program, Cambridge, Mass., 1972.

94. Echigo, R., Nishiwaki, N., and Hirata, M. "A Study on the Radiation of Luminous Flames." 11th Symposium (International) on Combustion, The Combustion Institute, 1967, p. 8.

95. Tan, H.S. and Lampe, F.W. "The Reaction of Ethyl Radicals with Nitric Oxide." J. Phys. Chem., 76, 23, 1973, p. 3303.

96. Ahumada, J.J., Michael, J.V., and Osborne, D.T. "Pressure Dependence and Third Body Effects on the Rate Constants for H + O_2, H + NO, and H + CO." J. Chem. Phys., 57, 9, 1972, p. 3736.

97. Kurylo, M.J. "Absolute Rate Constants for the Reaction $H + O_2 + M \rightarrow HO_2 + M$ over the Temperature Range 203 - 404°K." J. Chem. Phys., 76, 24, 1972, p. 3518.

98. Taylor, R.L. and Bitterman, S. "Survey of Vibrational Relaxation Data for Processes Important in the CO_2-N_2 Laser System." Revs. Modern Phys., 14, 1, 1969, p. 26.

99. DeMore, W.B. "Pressure Dependence and Mechanism of the Reaction of Atomic Oxygen and Carbon Monoxide." J. Chem. Phys., 76, 24, 1972, p. 3527.

100. Hartley, D.B. and Thrush, B.A. "The Rates of Elementary Processes in the Chain Reaction Between Hydrogen and Oxygen. III." Proc. Roy. Soc. (London), Series A, Vol. 297, Mar. 21, 1967, pp. 520-533.

101. Mellor, A.H. "Current Kinetic Modelling Techniques for Continuous Flow Combustors." Emissions from Continuous Combustion Systems, Ed. Cornelius, W. and Agnew, W.G., Plenum Publ. Co., 1972.

102. Lefebvre, A.H. "Design Considerations in Advanced Gas Turbine Combustion Chambers." Combustion in Advanced Gas Turbine Systems, International Propulsion Symposium, College of Aeronautics, Cranfield, Pergamon Press, 1967, p. 3.

103. Lefebvre, A.H. "Factors Controlling Gas Turbine Combustion Performance at High Pressure." Combustion in Advanced Gas Turbine Systems, International Propulsion Symposium, College of Aeronautics, Cranfield, Pergamon Press, 1967, p. 211.

104. Lee, K., Thring, M.W., and Beer, J. "On the Rate of Combustion of Soot in a Laminar Soot Flame." Comb. and Flame, 6, 1962, p. 137.

105. Fenimore, C.P. and Jones, G.W. "Oxidation of Soot by Hydroxyl Radicals." J. Phys. Chem., 71, 1967, p. 593.

106. Baulch, D.L., Drysdale, D.D., and Lloyd, A.C. "Critical Evaluation of Rate Data for Homogeneous, Gas-Phase Reactions of Interest in High Temperature Systems." Leeds Univ. (England) Reports, Nos. 1-5, 1968-1970.

107. Lavrendeau, H. "The Thermal Decomposition of Nitric Oxide and Nitrogen Dioxide." Univ. of Cal. (Berkley), Rep. TS-72-4, 1972.

108. Fletcher, et al. "The Control of Oxides of Nitrogen Emission from Aircraft Gas Turbine Engines." Vol. 1, Program Description and Results, Rep. FAA-RD-71-111, 1, 1971.

109. Kondratiev, V.N. "Rate Constants of Gas Phase Reactions." Office of Standard Reference Data NBS, Washington, 1972.

110. Jenson, D.E. and Jones, G.A. "Gas Phase Reaction Rate Coefficients for Rocket Applications." Rocket Prop. Estab. (England), RPE-TR-71-9, 1971.

111. Browne, W.G., Porter, R.P., Verlin, J.D., and Clarke, A.H. "A Study of Acetylene-Oxygen Flames." 12th Symposium (International) on Combustion, The Combustion Institute, 1969, p. 1035.

112. Clyne, M.A.A. and Thrush, B.A. "Reaction of Hydrogen Atoms with Nitric Oxide." Trans. of the Faraday Soc., 57, 1961, p. 1305.

113. Bulewicz, E.M. and Sugden, T.M. "Flame Photometric Studies of Reactions Induced by Nitric Oxide in Hydrogen-Oxygen-Nitrogen Flames - 1. Catalyzed Recombination of Atomic Hydrogen and Hydroxyl Radicals." Proc. Roy. Soc., A, Vol. 277, No. 1369, 1964, pp. 143-145.

UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)* Arnold Engineering Development Center Arnold Air Force Station, Tennessee 37389	2a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED 2b. GROUP N/A

3. REPORT TITLE

A LITERATURE REVIEW ON TURBINE COMBUSTOR MODELLING AND EMISSIONS

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*
Final Report - July 1, 1972 through March 31, 1973

5. AUTHOR(S) *(First name, middle initial, last name)*

I. T. Osgerby, ARO, Inc.

6. REPORT DATE November 1973	7a. TOTAL NO. OF PAGES 39	7b. NO. OF REFS 113

8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S) AEDC-TR-73-163
b. PROJECT NO	
c. Program Element 65802F	9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)* ARO-ETF-TR-73-103
d.	

10. DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES Available in DDC	12. SPONSORING MILITARY ACTIVITY Arnold Engineering Development Center, Air Force Systems Command, Arnold Air Force Station, Tenn. 37389

13. ABSTRACT

The rapidly growing body of literature on turbine combustor modelling is reviewed. The analytical models are presented and discussed with particular emphasis placed on their ability to predict gross operating characteristics as well as pollutant emission levels. Comparison is made between theory and engine and laboratory experiments showing the general inaccuracies of current models. A suggestion for improvement of the best available model is made, and areas for fundamental research are pointed out.

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
reviews						
combustion chambers						
turbine engines						
models						
exhaust gases						
emission						
air pollution						

1 Combustion chamber -- Modeling

2 " " -- Pollution

3 Turbine engines -- "

4 Exhausts -- "

AFSC
Arnold AFS Tenn