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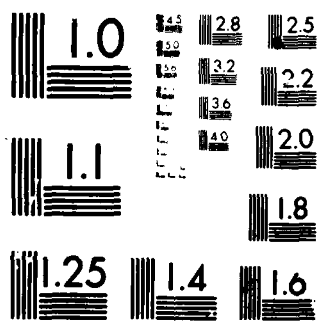

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AGARD ADVISORY REPORT No. 153

Technical Evaluation Report on the Propulsion and Energetics Panel 54th (B) Meeting on Combustor Modelling

NORTH ATLANTIC TREATY ORGANIZATION

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NORTH ATLANTIC TREATY ORGANIZATION

ADVISORY GROUP FOR AEROSPACE RESEARCH AND DEVELOPMENT

(ORGANISATION DU TRAITE DE L'ATLANTIQUE NORD)

AGARD Advisory Report No.153

TECHNICAL EVALUATION REPORT

on the

PROPULSION AND ENERGETICS PANEL 54th (B) MEETING

on

COMBUSTOR MODELLING

by

D. Dryburgh and R.B. Edelman

CONTENTS

This Advisory Report was prepared at the request of the Propulsion and Energetics Panel of AGARD.

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TECHNICAL EVALUATION REPORT

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1. INTRODUCTION

The 54th (B) Propulsion and Energetics Panel Specialist's Meeting on Combustor Modeling was held at DFVLR, Cologne, Germany, from 3-5 October 1979.

The objectives of the meeting were to assist manufacturers in the selection and justification of adequate theoretical models and to provide researchers with knowledge on realistic types of combustors and on the experimental conditions under which their theoretical models should be validated. The meeting provided a forum for comparing the models and methods used in turbine engines with those applied in non-aeronautical circles. The conference program was arranged by a committee under the chairmanship of M. l' Ing. en Chef Pianko.

There is a current critical need facing combustor designers and developers to meet more exacting requirements on efficiency, emissions, uncertainties of fuel availability and, of course, constraints on development costs and development time. The historical approach to the design of combustors has proven to be inadequate in effectively supporting the designer in meeting the stringent requirements imposed on developers by the emergence of these performance and economic constraints. Combustor modeling, on the other hand, is clearly emerging as a viable approach in terms of providing a new set of tools in support of the designer in effectively meeting these constraints. It was, therefore, a particularly appropriate time to hold a meeting on this topic. Work was sufficiently far advanced for the potential of modeling techniques to be demonstrated, though many problems remain to be solved and priorities for these need to be indicated.

There were 24 papers presented at the meeting and these were drawn from various sectors including manufacturers, supporting industry, university and government research facilities, some of which were combined investigations. The resulting set of modeling contributions covers a wide spectrum of relevant topics and levels of sophistication.

It was the wish of the Panel that this Technical Evaluation Report be written so as to express clearly the separate points of view of the manufacturer and of the research worker, and the Panel recognized that in some areas these might differ. The two main sections of this report have, therefore, been written in this way. Section 2 is a common one, classifying the content of the papers and creating a structure which the next two sections follow. Section 3 contains an overall review of the papers. Section 4 deals more specifically with those topics which the manufacturer regards as of great importance. Section 5 follows the same layout but is written from the point of view of a research worker. The final two sections, 6 and 7, are again common and contain the conclusions and recommendations.

2. CLASSIFICATION OF PAPERS

The papers presented at the meeting have been analyzed and classified in two ways - by topic and by dimensionality of the model used.

Table 1 gives a list of key words for topics or techniques of importance in combustor modeling. Against each is entered the reference number of those papers in which the technique plays a significant role. A distinction has been drawn between the application of an existing technique and the 'theoretical development' of a new one. It will be seen, for example, that no new methods of predicting flow patterns or turbulent transport were put forward at the meeting but that many papers employed existing methods for such calculations, some of them to investigate the effect of some aspect of another element of the model. It must be emphasized that many key words, such as 'flow patterns' cover a wide range of methods, e.g. 1-, 2-, or 3-D models or transient methods of flow calculation.

This method of classification exposes two significant features of the papers presented. In the first place, although there were many interesting examples of the application of modeling, relatively few new ideas were proposed. (More of these referred to somewhat less exploited aspects of turbulent/chemistry interaction and one further paper dealt with several aspects of fuel chemistry.) In the second place, there is great reliance on a relatively few basic modeling tools. Further investigation reveals that a 2-D finite difference calculation of the flow pattern, with the k-ϵ turbulence model is used in many applications.

TABLE 1. PAPER CLASSIFICATION - MODEL ELEMENTS

COMBUSTOR MODEL ELEMENTS	APPLICATIONS	THEORETICAL DEVELOPMENT
Aerodynamics		
Flow Patterns	Ref. 2,3,4,5,6,7,8,10,14,16,17,19,24	
Turbulent Transport	Ref. 2,3,4,5,6,7,8,10,14,16,17,19	
Multiphase Flow	Ref. 2,3,10,22	
Premixed	Ref. 13,14,15	
Diffusion	Ref. 2,3,4,5,7,8,10,16,17,19	
Supersonic	Ref. 8	
Fuels		
Physical Properties		
Volatility	Ref. 2,3,10,22	
Chemical Properties		
Equilibrium	Ref. 16,17,22	
Pyrolysis	Ref. 12	11
Vapor Phase	Ref.	11
Oxidation	Ref. 2,4,8,10,13,14,16,21,23,24	11,12
Kinetics	Ref. 2,5,8,10,13,14,17,19,21,22,24	11,12
Soot Formation	Ref.	11
Soot Consumption	Ref.	11
Fuel Bound Nitrogen	Ref.	11
NO_x	Ref. 2.4.13.19,21,22,23,24	11
Turbulent Interactions		
Turbulent/Combustion Interaction	Ref. 3,8,10,14,19	2,4,5,7,13
Radiation	Ref. 2,9,10,16,19	
Instabilities/Transients	Ref. 14,15	

Table 2 classifies the papers according to the dimensionality of the model used: this is a reflection of the complexity of the flow under investigation. Briefly the model types are:

Empirical--Relations of a fairly simple nature, usually in the form of correlations of experimental data, but where the functional form of the relation has no clear physical basis.

Semi-Empirical--Relations where the functional form can be defined by physical reasoning but with constants determined from this data.

O-D (Zero-dimensional models)--Where there is no spatial variation in the region under study or where such variations are neglected.

Multidimensional Models

1-D 2-D 3-D	models of increasing complexity, with variation in 1, 2, or 3 space dimensions
1-DT 2-DT	unsteady flow in 1 or 2 space dimension

Hybrid--Various combinations of the above types

Table 2 shows that the most popular model is a 2-D one, almost entirely for a cylindrical flow with a finite difference solution algorithm and a k-ϵ turbulent transport model. There is comparatively little 3-D modeling but quite a few O-D and 1-D cases.

TABLE 2. PAPER CLASSIFICATION - MODEL DIMENSIONALITY

MODEL TYPE	APPLICATION	THEORETICAL DEVELOPMENT
O-D..............	Ref. 2,11,13,15,21,14............	....
1-D..............	Ref. 12,13,16,21,24..............	....
2-D..............	Ref. 3,4,5,6,7,8,9,10,16,17,19....	....
3-D..............	Ref. 2,3,8,14....................	....
1-DT.............	Ref. 15..........................	....
2-DT.............	Ref. 14..........................	....
Empirical........	Ref. 22,23.......................	....
Semi-Empirical....	Ref. 22,23.......................	....
Hybrid...........	Ref. 1,2,8,11,13,16,21,24........	....

Table 3 lists the papers that are of a survey nature covering the gas turbine developers' needs, radiation and furnace modeling, respectively.

TABLE 2. PAPER CLASSIFICATION - SURVEY TYPE

Subject	Reference
Primary	
Aircraft Gas Turbines..................	1
Radiation Models.......................	9
Alternate Fuels........................	11
Secondary	
3-D Modeling...........................	2
Supersonic Combustion Modeling.........	8
Furnace Modeling.......................	16

As a general rule it might be expected that the simpler type of flow under consideration, the greater the degree of dimensionality that can be exercised with respect to the evaluation of new developments in chemistry, radiation, turbulence, etc. This approach is the very commendable one of developing and validating a new aspect of the model in a simple flow and then applying it, tentatively at first, to more complex types of flow. Section 3 gives a general evaluation of the papers presented at this meeting. In Section 4 and 5 the implications of the work presented at this meeting relevant to the manufacturers' and users' needs and to researchers are discussed, respectively.

3. EVALUATION OF PAPERS - GENERAL

The evaluation of the papers presented at the meeting starts with a review of the survey papers and this sets the scene for a more detailed discussion of the material from the other papers. Empirical models will be considered first since they are the simplest and most familiar. They are followed by zero-dimensional models, mostly of the stirred reactor type, and then, with increasing complexity, one-dimensional models and, finally, the more detailed two- and three-dimensional models. This scheme takes in most of the papers but two further subsections cover unsteady flows and methods of obtaining quantitative data from airflow experiments for input, usually, to reactor network models. This approach to the review is not without its disadvantages, as a few papers appear several times in different subsections, but it does enable the technical problems common to a number of papers to be discussed as a whole.

3.1 Survey Papers

Three of the papers, by Gastebois [1] , Bartelds [9] , and Edelman, Turan, Harsha and Blazowski [11] can be regarded as survey papers.

Gastebois' paper, which has already been mentioned, considered a manufacturer's requirements for a modeling procedure. His conclusions might have been regarded as rather pessimistic by some of the other participants as Gastebois felt that the two- and three-dimensional models would always be too large and too complex for routine use and in his view, reactor-network, or modular models would be the largest to which industry would be likely to aspire.

Bartelds' review of radiative heat transfer [9] was a comprehensive and understandable account of a complex subject. The paper is well organized in terms of the coverage given to the fundamental aspects of absorption and emission processes and of the practical aspects involved in the incorporation of these mechanisms in the modeling of the radiation exchange process. Multiflux and continuous intensity distribution transport models were analyzed and evaluated primarily in the context of steady axisymmetric flows. There appeared to be two possible approaches: the first, applicable when the gas is at a more or less uniform temperature, uses one of the multiple grey gas models to obtain the emissivity and a zone method to calculate the net radiant flux to the wall. Spectral methods for the determination of emissivity are more fundamental and accurate when the gas temperature varies, could be used for a variety of fuels and could include the effects of soot. They are, moreover, better suited to finite difference models where the radiation is treated by a flux method.

The growing likelihood that future gas-turbines will have to burn fuel of more variable quality poses many problems for the designer. Nearly all the processes which take place in the primary zone are affected by the fuel placement and such properties as viscosity and volatility. Paper [11] on the characterization of alternative fuels by Edelman and his co-workers reviewed these and other aspects. Most of the paper, however, was devoted to an account of recent work on the formation and oxidation of soot. This complex process, if broken down into a series of steps and reaction rates for each, could be determined by suitably designed experiments. The fuels studied appeared to fall into three classes for sooting ability: ethylene and other aliphatic compounds produced least, while toluene and other compounds with a single aromatic ring formed appreciably more. Fuels with more than one aromatic ring, such as naphthalene, came in a separate category with a very high production of soot.

The contribution of this paper, when taken in conjunction with that of Bartelds, could be quite significant and opens up the possibility of modeling soot production in the primary zone and hence the smoke emission from the combustor and the radiative heat transfer to the walls.

Three other papers can be regarded to some extent as reviews, although they are primarily directed toward specific applications of selected techniques.

The paper by Swithenbank, Turan and Felton [2] described the use of a 3-D program to make predictions with which to compare with measurements obtained from a model gas turbine can combustor. In addition, a method of including evaporation and mixing in stirred reactor theory and an experimental tracer technique for identifying reactor volumes were described. The approach involving the application of a 3-D code with simple two-step kinetics to delineate flow regions characterizable by reactor modules enables one to then treat these regions with more complete chemistry. This is particularly significant in terms of providing a variable systematic approach to the analysis of complex flows with complex chemistry such as that associated with pollutant emissions, as well as the formation and disposition of soot.

Drummond, Rogers and Evans of NASA [8] described the types of models required for the design of a supersonic-combustion ramjet and reviewed the progress that has been made in the development of the flow field models necessary to characterize the complex interactions encountered in flows containing shock waves. Application was made of models of varying levels of sophistication depending on the flow region under investigation. The models spanned the spectrum of 1-D, 2-D, and 3-D and included parabolic, elliptic and hyperbolic types.

Michel, Michelfelder and Payne [16] described the application of 0-, 1- and 3-dimensional models to the calculation of the wall heat flux (radiative plus convective) for several of the IJmuiden furnaces. The type of model had to be matched to the characteristics of the furnace and there was quite an impressive demonstration where all the models were applied to the same set of measurements and the improvements in accuracy with increasing dimensionality of the model was quite clear. This paper illustrated the significance of selecting the level of model sophistication to match the type of information that is relevant to the particular problem.

Items from these papers will be discussed more fully under the appropriate headings below.

3.2 Empirical and Semi-Empirical Models

Two papers, both in the final session, showed that there was still much to be learned from a simple extension of the methods that have been used for many years by the 'practical combustion engineer'. Mellor [22] based his approach on a series of characteristic times which control the processes taking place in the combustor. Some of these times, for example those for evaporation and several turbulent mixing times, were evaluated from reaction rate formulae. He showed some quite effective correlations for the stability of different types of flames and for CO and NO_x emission rates. Odgers [23] in turn showed that there were many 'design rules' which could be used for aspects of combustor performance ranging from stability to the calculation of cooling air requirements, exit temperature distribution and emissions level.

These models are simple, cheap in terms of computer time, easy to use, and are well suited to the evaluation of a large number of possible designs. However, their validity is rather doubtful when a modification of an existing design does not fit the original data base or when a radical new approach is being tried. Some designers prefer to regard these rules as giving an estimate of the current state-of-the-art while on fundamental grounds there is little basis to regard these correlations as more than fortuitous.

3.3 Stirred Reactor Models

Because of their simplicity and the inherent assumption of large scale homogeneity, stirred reactors can be an effective way of representing the chemical processes in highly backmixed regions of the combustor. Swithenbank [2] described a method of including droplet evaporation rates and fuel-vapor mixing rates in the normal formulation of a stirred reactor. The incorporation of chemical kinetics resulted in quite a complex system of equations for which special methods of solution had to be devised. This technique was applied to a specially designed combustor in which the reactor volumes could be easily defined and it showed quite good agreement for the NO_x and CO concentrations.

Stirred reactors are popular vehicles for testing other modeling hypotheses, particularly those based on global reaction rates. Experimental stirred reactors can be used to determine global rate constants, for example, for fuel pyrolysis and soot formation - Edelman [11] . They can also be connected together to form one- and two-dimensional arrays and some of these will be discussed in the next subsection (Pratt [13] and Krockow, Simon and Parnell [21]).

3.4 One-Dimensional Models

One-dimensional models are not greatly used, perhaps because few real combustors are one-dimensional. However, such flows are easy to compute and quite complex chemical kinetic schemes can be evaluated in detail.

Dryer and Westbrook [12] showed that, even for a simple type of fuel like methanol, the complete reaction scheme includes at least 84 separate reactions. The combustion of more complex hydrocarbons could be characterized by two-step global reactions or by quasiglobal reactions. In the second case, the fuel can be broken down into simple molecules, perhaps CO, H_2, CH_4, etc., and the oxidation of these intermediate species can be considered in detail. The method described took no account of the effects of turbulence on the reaction rate, and if the constants of the global step are evaluated from measurements under conditions where sufficient care was not given to minimizing unmixedness, the results may well not be applicable in a situation with a different or varying level of turbulence.

Michel, Michelfelder and Payne [16] showed some success in the application of a one-dimensional model to a long furnace where the flow was reasonably one-dimensional, but in other cases this simple treatment was not so good.

In certain treatments of unmixedness the flow is represented by a suitable combination of plug flow and stirred reactor phenomena, i.e. reactions in series and in parallel. There were two interesting papers in this area [13] ,[21] . Pratt's paper [13] on coalescence-dispersion modeling was based on a stochastic approach in which the reactor was regarded as an assembly of 'turbules' in each of which the chemical rate was integrated step by step. Mixing is simulated by choosing two turbules at random, averaging their properties and replacing them. The selection of turbules leaving the reactor is also made randomly. The method was applied with some success to premixed flames, where in the few cases that were evaluated, the results appeared to agree better with experiment than conventional stirred-reactor theory.

Krockow, Simon and Parnell [21] also used a probabilistic method for their combustor calculations. Their model is a development of Fletcher and Heywood's ideas where there is assumed to be a Gaussian distribution of fuel-air ratio and an exponential distribution of residence time in the primary zone. Each element starts to react in the primary zone and continues as it passes through the secondary and dilution zones to the combustor exit. The equations can be integrated to give the species concentrations along the chamber. Six hundred 'turbules' were considered, corresponding to all combinations of 30 mixture strengths and 20 residence times, and the results were combined to give the mean compositions of all species down the chamber. The fuel-air ratio at the primary zone exit was measured and used to establish the parameters of the mixture strength distribution. This work, simple though it was in conception, was well presented and seemed to be quite successful in predicting levels of CO, HC and NO_x at the combustion chamber exit. The effect of geometrical changes to the flame tube on pollution levels could easily be assessed.

3.5 Two- and Three-Dimensional Models

More than half the papers presented used one of these models at some stage. They are not essentially different and are considered together. The 3-D models are more complicated but both try to give spatial resolution in the combustion chamber. These models are fundamental by nature, they should be applicable to different geometrical shapes, and they should allow the many aspects of combustor performance to be viewed from a detailed and consistent base.

These models have perhaps five separate aspects:

1. Method of solution of the equations of motion
2. Turbulence model
3. Droplet model (if liquid fueled)
4. Combustion model (chemistry)
5. Radiation

Almost all the papers used the same (finite difference) method of solution based on the work of Spalding and his co-workers, and almost all used the same turbulence model ($k - \epsilon$). The assumptions for droplet evaporation are very similar and, where radiation was included, the treatment was along the same lines. The only area that showed a large degree of diversity was the modeling of the combustion process in the presence of turbulence. This is one of the frontiers of research and poses difficult and fundamental problems with current activities being in the formative stages.

3.5.1 Turbulent/Chemistry Interaction

In turbulent flows the rate at which the reactants are mixed by the turbulence can be slower than the chemical rate governing heat release. The representation used for chemical kinetics therefore has to be extensively modified for turbulent flows to account for fluctuations in temperature, etc., and many different approaches have been tried, the intention being to eliminate the least successful ones and concentrate on the others. The papers presented covered a wide variety of chemistry models and, since this is one of the most important problems facing combustor modelers, it is worth while discussing them in some detail.

Swithenbank, Turan and Felton [2] adopted the eddy break up (EBU) model. They reported good agreement with experimental velocity and temperature profile data obtained from a research combustor. Some discrepancy was observed with the species comparisons but since the numerical method required a large number of iterations for convergence, it was difficult to tell how much of the discrepancy with experiment was due to the EBU model and how much was due to the possible lack of convergence. The authors, however, used the 3-D finite difference model to set up a reactor network from the flow pattern and the combustion reactions were evaluated in well-stirred reactors.

Jones and McGuirk [3] assumed

1. A one-step reaction with the products in equilibrium particularly as regards the reactor

   $$CO + \tfrac{1}{2}\ O_2 \rightleftharpoons CO_2$$

2. The reaction was mixing-controlled

3. A beta-function pdf for mixture fraction

Their results showed fair agreement with experiment for a range of swirling and non-swirling flows, but there was room for quite a lot of improvement in the details.

Janicka and Kollmann [4] considered the rather simpler experiment of a jet of hydrogen burning in air. Their assumptions included:

1. Partial equilibrium chemistry with four two-body reactions in equilibrium and three three-body reactions kinetically and mixing controlled.

2. A joint pdf for mixture strength and reactedness which were assumed independent. A beta distribution was used for mixture strength and one with three delta-functions for reactedness.

The results showed quite good agreement with measurements out to about 80 jet diameters, and the authors were able to explain the errors in terms of shortcomings of the assumptions. A better approach was outlined which involved solving for the shape of the joint pdf but it had not been evaluated.

Eickhoff, Grete and Thiele[5] adopted a rather simpler approach in their study of natural gas flames. They assumed:

1. A single step fast reaction with quenching at mixture strengths greater than twice stoichiometric

2. A 'clipped gaussian' form of pdf

3. A turbulent closure which modeled the triple correlation $\overline{\rho'u'v'}$ in terms of the Reynolds' stress $\overline{u'v'}$ and the density gradient

4. A modification of the shear-stress relation for polar geometry

The last two assumptions introduced two constants whose values had to be determined from experiment and the authors were able to show that values could be found which predicted the isothermal mixing of gases of different density as well as the combustion of free jet and confined natural gas flames. The main errors were in the radial profiles at over 60 diameters from the entry.

Whitelaw and el Banhawy [10] used quite a simple chemistry model but their main interest was in the effects of changing assumptions for the droplet model.

Gamma, Casci, Coghe and Chezzi [17] considered a methane diffusion flame with swirl in a confined burner and tried to analyze it with two reaction schemes:

1. Instantaneous reaction, mixing controlled

2. Global reaction with mixing and kinetic control

They compared the predictions with their own measurements and found that the second scheme was perhaps a little better for velocity while the first was better for temperature. Both were in error near the injection plane.

Michel, Michelfelder and Payne [16] used a very simple chemistry model for their calculations of the Ijmuiden furnace. However, their principal interest was in the calculation of the radiant heat flux rather than the species composition and pollutant formation.

Guenot and Ivernal [18] applied a 2-D model to the case of a combustor using air enriched with oxygen. The high temperature achieved meant that dissociation of the products had to be taken into account, but, apart from a method developed to handle the temperature-mixture strength relation, the model was substantially the same as many of the others. It assumed:

1. A fast global reaction

2. A double delta pdf for the mixture strength

Paauw, Stroo and von Koppen [19] analyzed the results of a natural-gas fired furnace at Delft according to three chemical models:

1. Frozen composition (mixed is burnt)

2. Equilibrium composition

3. Partial equilibrium - an observational modification of the equilibrium composition at fuel-rich conditions

A 'clipped gaussian' pdf was assumed and its parameters were determined by experiment and a non-gaussian pdf for mixture fraction was deduced from the chemistry model and used to relate the time-mean reaction rates to the time-mean species concentrations. Detailed comparisons with experiment gave quite good agreement for both the equilibrium and partial equilibrium models. The partial equilibrium method was preferred because it gave better agreement with the observed pdf. If this approach was to be used in other situations, the partial equilibrium model might have to be modified for other fuels and some means of relating the standard deviation of the temperature to other characteristics of the model would have to be found.

Varma [7] presented an interesting theoretical paper in which he pointed out that assumed forms of pdf can lead to physically unrealizable consequences. He discussed the various constraints which affect the modeling of second and third order correlations and showed how these could be satisfied using pdf's constructed from delta functions. This enabled the second order moment equations to be solved in closed form with no further modeling assumptions.

Elbahar and Wittig [6] used a 2-D model to calculate the temperature profile at the exit from an annular combustor where dilution air was injected through a row of closely-spaced holes. A true 3-D treatment would be required, however, when the jets remain separated over an appreciable proportion of the combustor height, as is the custom in many practical dilution systems where such a configuration gives more rapid mixing and hence a shorter combustor.

3.5.2 Droplet Model

The Whitelaw and el Banhawy paper [10] was the only one specifically concerned with droplet behavior and used a more detailed model than either Jones [3] or Swithenbank [2], both of whom assumed that droplets followed the flow. Swithenbank showed that this assumption was not satisfied for the larger droplets and suggested than an iterative procedure could be employed to achieve coupling with the gas phase flow.

Whitelaw and el Banhawy solved the droplet equations of motion in a given flow field and then iterated between the droplet motion and the flow equations. Their work included the effect of varying the number of droplet size ranges. For sprays confined to a small region, particularly if there was also intense turbulent mixing, only about five size ranges were necessary, whereas, for longer flames with slower mixing, 20 or more might be needed.

The interaction between turbulence and droplet dynamics was not discussed in any of the papers.

3.5.3 Radiation

The flux method described by Bartelds [9] was the most appropriate for a finite difference calculation and was used by most of the authors who included radiation [2], [10], [19]. However, Michel, et al [16] was the only paper concerned primarily with radiant fluxes and they applied both zone and flux methods.

As in the case of droplet dynamics, the interaction of turbulence with radiation transport was not discussed in any of the papers.

3.5.4 Numerical Methods

None of the papers devoted significant attention to this vital aspect of modeling procedures. The problems in terms of the papers presented are those of convergence and grid-independence. Swithenbank's model showed a mass imbalance of about 2% of the inlet mass flow, even after 240 interactions. Whitelaw [10] and Paauw [19] both investigated the grid-independence of their solutions and showed how the predictions could be improved by ensuring good grid resolution in the sensitive areas of the flow. Paauw found that too coarse a grid led to an underestimate of the rate of turbulence generation and hence to a larger recirculation volume.

Another point which was mentioned in Whitelaw's paper [10] and which also appeared in the discussion of some of the other papers was the importance of knowing all the boundary conditions accurately when evaluating a 2- or 3-D model of a combustion chamber.

3.6 Unsteady Flows

Two papers looked into aspects of unsteady flows: the first, by Hirsinger and Tichtinsky [14] used a finite difference formulation and a simple chemistry model to demonstrate how ignition spread behind a baffle in an afterburner. They showed first, how a steady state non-combusting flow could be established and then how the flame spread out from an ignition source located in the center of the recirculation zone downstream of the baffle. From a mathematical point of view, there is not very much difference between an unsteady flow and the iterative approach to a steady one, and the ability to visualize the temporal development of the flow can sometimes be very useful. One of the disadvantages is the very large amount of computer output produced, but this was overcome in the presentation by effective use of computer generated movies.

A second problem looked at by the same authors was the flow from a feed annulus, through a hole into the primary zone of a combustor chamber. It was not so clear in this instance what the benefits of an unsteady approach were, but the final steady state showed the angle at which the jet entered the chamber and the flow it induced. No other paper presented touched upon the potential application of modeling procedures for isolated aspects of an overall design. There are many instances where models can be used in this way to give the designer or development engineer and the researcher a better understanding of what may happen in different circumstances. At their current state of development, models are capable of doing this and more emphasis could be placed upon such applications while models of the chemistry, for example, are being separately developed.

The second paper in this group was by Marble, Subbaiah and Candel [15] and it studied mechanisms for the amplification of acoustic waves by combustion processes in an afterburner. An integral relations technique was used to reduce the problem to a one-dimensional unsteady one in which the wave processes could be studied.

3.7 Experimental Input to Stirred Reactor Models

One of the major problems encountered in setting up a stirred reactor network to represent a practical combustor is to decide how the individual reactors shall be delineated and how they should be characterized in terms of volume, mixture strength and their interconnections with other reactors. Two papers touched upon this problem.

Swithenbank [2] described two approaches. The first was the use of a 3-D mathematical model to calculate the flow and divide the combustor volume into zones of approximately equal mixture strength and turbulence intensity. The other was based on an experimental technique whereby a salt tracer was injected into a water-flow model. At each injection position the tracer was injected as a series of pseudo-random pulses: correlation techniques were used to relate the detected and injected pulses and give the time lag and intensity of the detected signal.

Hebrard and Magre [24] described rather more conventional methods of analyzing measurements on different types of models and obtained results in a form suitable for use in setting up reactor networks. Water analogy and cold airflow rigs were used to determine flow patterns, reactor boundaries and residence times and work is in progress in devising methods for the automatic analysis of the data. Small, single-sector combustion rigs were used for efficiency measurements and pollution levels. NO_x was determined with a standard chemi-luminescence meter while a series of gas-chromatographs were used to obtain the concentrations of the other species.

4. EVALUATION OF PAPERS - THE MANUFACTURER'S POINT OF VIEW

4.1 The Use of Models in Industry

Modeling is primarily a tool for the designer of combustion chambers. It is an extension of his own understanding of combustion processes, though not a replacement for it. He can use models to investigate new ideas, understand the often complex relationships between the variables that are under his control, optimize a design to meet the conflicting requirements imposed upon the combustor and determine the sensitivity of the design to changes in the basic parameters. A variety of models are needed, ranging from simple rapid ones used at the conceptual design stage where many different possibilities have to be explored, through those of intermediate complexity used once a design approach has been decided, and culminating in the very elaborate and detailed models used to predict the behavior of a few remaining possibilities. This concept of a hierarchy of models was brought out by Gastebois [1] and Odgers [23] who both described how the different types of model could be used at successive stages of the design process, and by Michel [16] . Gastebois also pointed out that the development engineer should have an interest in combustor models. Since it is his task to make good the shortcomings of the initial design, and since time and cost can be even more important at this stage, this is an aspect that should not be overlooked. The research worker, too, relies heavily on models. Many of the papers presented, for example, most of those dealing with the turbulence/chemistry interaction, depended on airflow and turbulence models to enable comparison to be made with experiment.

Gastebois [1] gave a list of the six most important design parameters.

1. The distribution of air among the different zones of the combustion chamber
2. The pressure loss
3. Wall temperatures over the operating envelope
4. Stability (including ignition limits and relight capability)
5. Exit temperature traverse (pattern factor)
6. Emissions levels

The designer would like to be able to predict all of these with reasonable accuracy without having to test a complete flame tube or parts of it. All are interrelated to some extent and, apart from the emissions, all have been long standing requirements. The two great challenges today for the designer are emissions and alternative fuels which are responsible for most of the current interest in modeling. The requirement to reduce emissions, in some cases by a factor of 10 or more, has brought about a complete rethink of combustion chamber processes, while the need to consider alternative fuels, often with a high aromatic content, has ramifications in many areas, particularly those of stability and radiative heat transfer. Only one paper [11] dealt directly with fuel properties, though many were concerned with modeling the chemistry of pollution formation.

Odgers [23] gave a succinct statement of four of the cardinal principles of modeling:

1. Accuracy
2. Solution time
3. Simplicity and comprehensibility
4. Cost

To these can be added

5. Realism and generality

The the current stage of development of combustor modeling, accuracy is not always as good as might be desired but, if the significant physical phenomena are well represented, the model can still be used to gain an insight into the behavior of the combustor. If generality can be incorporated at a fundamental level, the model can be applied to a range of problems and, once it has proved its validity in one area, its extension to others should be a simple matter. Gastebois drew attention to the dangers of empirical models where parameter values had to be selected depending on the application.

4.2 Summary - From the Manufacturers' Viewpoint

At this point the manufacturer must look at the evidence that has been presented to him and at his own requirements, and he must try to decide what kind of combustor models he wants. This is not too easy a task as there were few tried and tested products on offer. There were many examples of modeling virtuosity which amply demonstrated the potential benefits of this type of approach but all too often these had to excuse their lack of accuracy by pointing to a long list of other problems for which a solution was still required.

It emerged quite clearly, however, that a series of models of different complexity are needed, the complexity of the model being related to the degree of refinement required in the calculations, and inversely related to the number of cases to be analyzed. Obviously the familiar, simple design rules are still necessary and the work of Mellor and Odgers should be followed up, its range of applicability determined and extended to include new requirements.

Something better is needed to enable the manufacturer to meet the conflicting requirements imposed on him by the energy crisis and the pollution legislation, and by the increased cost and extended time scale of trying to design tomorrow's combustors by the traditional methods. The research community offers two possibilities here - reactor networks and the more fundamental two- and three-dimensional finite difference methods. Gastebois [1] stated his preference for reactors because, in his view, 3-D models would be too large and complex for routine use. The purpose of the meeting, however, was to bring the manufacturer up to date with the progress of research and it showed that work on 2- and 3-D models has made great strides and is capable of giving quite encouraging results.

The proponents of reactor networks claim that their method is simple and easy to understand, that it is quick to run on a computer and that it can take account of the chemical reactions to a more detailed level than is practicable with a finite difference model. In response, the supporters of finite difference method point out that the simplicity is misleading, that there is a certain degree of arbitrariness in the way in which a particular combustor can be represented by a network of reactors, that reactors are limited to answering some questions on efficiency, pollution levels and possibly stability, and, finally, that the claim to handle chemistry better is spurious.

Swithenbank's derivation of the reactor equations to include droplet evaporation and mixing effects led to a very complex set of equations which required a specialized method of solution. Moreover, the underlying assumption of stirred reactor theory is that the mixing time is much less than the reaction time, whereas the applications of the 2- and 3-D models involved situations where the mixing rate was usually much slower than the reaction rate. The inability to model the turbulence/chemistry interaction which has assumed such importance in finite difference models should to an equal extent, prevent the accurate modeling of a stirred reactor.

The problems facing the supporters of two- and three-dimensional models are great, but, nevertheless, some of the results presented showed that the experimental results could be reproduced to quite good accuracy providing that sufficient attention was paid to the detail. This means a careful choice of grid to give solutions which are grid-independent and an adequate representation of the chemistry. The modeling of the turbulence/chemistry interaction is one of the most active research fields but there is, as yet, no accepted way forward. For simple hydrocarbon fuels, Eickhoff [5] and Paauw [19] had quite effective models which incorporated observational modifications of the flame behavior. These might, however, not be sufficiently general for use with other fuels. Janicka and Kollmann [4] had a more fundamental approach with a joint pdf of assumed form but it was applied to a very simple reaction scheme.

The methods of treating radiation appear to be well established and there is some hope that the kinetics of soot formation can be incorporated in these models, (Edelman [13]) and the correct gas properties deduced.

There was a surprising acceptance of the numerical procedures and the turbulence model used in many of the methods. These are fundamental to any progress and the requirements to give an accurate grid-independent solution still have to be established.

There are some topics not touched upon at all but which will have to be investigated before two- and three-dimensional models can be applied to actual combustion chambers. The most important is the problem of geometry; all the work presented was carried out in very simple geometries and the introduction of real shapes will require modifications to the numerical method of solution which may affect its accuracy and rate of convergence.

There are other topics, again barely mentioned, where models could be applied now to good effect. Many are quite simple and involve only isothermal flows: the diffuser between the compressor outlet and the combustion chamber is an important component as it has to divide the flow in a stable fashion and with the minimum of loss between the inner and outer annuli and the head of the chamber. In the annulus itself there are often puzzling features of the flow which ought to be amenable to a modeling approach as should be the behavior of holes of differing shape and with different kinds of plunging or chutes. The list of such applications is endless and is not confined to the combustion chamber. An elliptical 3-D program is a very powerful tool that has not previously been available.

The meeting has shown that combustor modeling as a subject has reached maturity. It has gone too far and too successfully to think of stopping or going back. The potential benefits have been amply demonstrated and the principal problems exposed, though general methods are not obvious in every case. The next stage of development must concentrate systematically on finding solutions and in general improving accuracy. The enthusiasm and inventiveness of those engaged in this endeavor is a good assurance that progress will continue, that further aspects of combustor performance will be brought within their compass and that the benefits being sought will be achieved.

5. EVALUATION OF PAPERS - THE RESEARCH POINT OF VIEW

5.1 The Development and Use of Models by Researchers

The requirement to develop high performance propulsion, power generation and other energy conversion devices has created a need for research on combustion problems in advanced systems. The demand for improved performance is complicated by the uncertainty in fuel supplies, the possibility of alternate fuels, and the requirement for pollutant emissions control. Many of the problems arising out of these constraints are current while others are of longer range. The research that is required in addressing these problems needs to span the range from fundamental studies to applied research that includes the development of comprehensive engineering models. This process of model development should follow a systematic approach by which each relevant mechanism is treated separately and then coupled to form the model of the combustor. This modular development should be attractive to the designer because it admits to a building block approach while the researcher inherently adopts this view in developing a fundamental understanding of each relevant process.

The meeting having been largely devoted to combustor modeling represents a type of culmination of research through the integration of various theoretical descriptions of the component processes into a hierarchy of combustor model sophistication. While the papers taken as a whole touched upon many of the important mechanisms relevant to combustor modeling, few devoted any attention to the significance of the lack of depth of understanding with respect to many of the component processes. There are certain phenomena that were not addressed at all. In isolating the phenomena of potential importance it is useful to consider the various problem areas in categories that relate to the basic issue of combustor modeling. These categories include fuel preparation, combustion chemistry, combustion dynamics and finally, combustor modeling.

Fuel preparation in the present context includes the processes of fuel injection, atomization and droplet consumption. Spray characteristics are dependent upon the liquid viscosity, volatility and surface tension and for alternative fuels these properties can be significantly different from those of conventional fuels and can lead to excessive droplet life times. The effects of injector characteristics on the combustion process would be useful to know in order to provide guidance on injector requirements. Understanding primary and secondary atomization would help to support injector design to meet these requirements. Droplet consumption was treated in the usual diffusion controlled limit applicable to the evaporation of conventional, volatile fuels [1 and 10]. There was no discussion of liquid phase reactions nor of the formation of particulates out of the liquid phase that can be expected to pose a problem with certain of the more viscous, less volatile alternative fuels.

Combustion chemistry has traditionally been characterized by one or two step kinetics which have served to account for certain of the effects of finite rate heat release. Current concerns on altitude relight in aircraft gas turbine in particular, and on the fate of CO, for example, and of the formation and consumption of particulates in general, indicate the need for a better understanding of the role of intermediate species. Quasiglobal modeling [11] represents a step in this direction while detailed modeling is developing [12] and represents an important activity with its potential to provide a more basic understanding of kinetics processes in general.

Combustion dynamics includes such phenomena as the coupling of the aerodynamics and the chemistry. This particular interaction was discussed in several papers whereas other important turbulent interactions were not discussed at all, most notably the droplet and radiation coupling to the turbulent fluctuations. This development step in arriving at combustor models was not discussed as such in the meeting yet it represents a significant research area. The development of models through iteration with a set of generic, canonical, flows has not received the attention required to first validate combustor models on the simplest of flows.

Combustor modeling represents the final step involving the tying together of the physical and chemical elements necessary to characterize practical combustors whether they are conceptual or already exist.

5.2 Summary - From the Researcher's Viewpoint

The meeting provided the researcher with some information on the practical problems being encountered in the development of combustor models and some practical information on actual combustors and operating conditions. A notable point is that the hierarchy of models ranging from 0-, 1-, 2-, and 3-dimensional types are not only of interest to the manufacturer but are ideally suited for the researcher striving to develop a better understanding of the unit processes. The multidimensional models are also of equal importance to the reseacher since they serve as research tools in the development of fundamental information on physical and chemical mechanisms that are encapsulated by the full Navier-Stokes type of equations.

The results presented at the meeting show that a concerned model validation effort is required. At the same time it is clear that research is needed on spray combustion, chemical kinetics, and on the various turbulent interaction processes. Well defined and well characterized experiments are needed to accompany model development of each of the unit and coupled processes. Initial and boundary conditions must be carefully defined and measured. This should include the scales as well as the intensity of turbulence. The models themselves should be used in concert with the definition and performance of experiments. In this regard virtually no sensitivity studies were covered in the papers and this type of information is relevant to establishing some guidance on the relative importance and accuracy requirements of the various measurements. Similarly, sensitivity studies on the assumptions made in characterizing each of the mechanisms contained in the models need to be carried out along the way in order to keep the research priorities in perspective on a continuing basis. As more emphasis is placed on multidimensional models numerical accuracy will become of even more concern. If numerical inaccuracies mask the physical and chemical models being developed the effort will become counterproductive. There was some evidence of this problem in the papers presented at the meeting. Geometry was another aspect of the numerical methodology that did not receive attention at the meeting. Methods for the treatment of curved geometries need to be exploited and further research is required to develop the means for treating arbitrary geometries more accurately than was done in the work presented at the meeting.

Despite the shortcomings indicated here certain very fruitful approaches emerged from this meeting. The hierarchy of models and various combinations of these to construct modular models are valid tools for conducting research on individual and coupled processes which can then be readily adapted to practical situations while putting minimum strain on computer requirements. That the gap between research and application is shrinking is demonstrated by the work reported by Mongia, References 14, 15, and 16 of Mellor's paper [22] . This work involved an interrelated 3-D combustor model/hardware design program. The results of fabrication and testing successfully demonstrated the use of modeling in hardware design. It seems clear that with a cohesive approach to further the integration of basic and applied research coupled with the user's needs that combustor modeling will indeed lead to practical design tools.

6. CONCLUSIONS

1. There is general agreement that, from the point of view of both technical and economic factors advances in combustor development will benefit from the application of modeling techniques.

2 The modeling process can provide the designer with a set of tools which he can use to investigate the effect of parameter variations on all aspects of combustor performance during the design and develop- phases.

3. A hierarchy of models is evolving ranging from semi-empirical correlations, useful mainly at the conceptual design stage, to three dimensional computer programs applicable to the detailed design and evaluation stages.

4. The majority of the papers presented were applications demonstrating the power of the various levels of modeling. The results indicate a requirement for the systematic validation of the predictions and at the same time suggested areas where further model development is required.

5. The results presented in the papers suggest the following subjects for further research:

   Turbulent/combustion interaction

   Spray dynamics, including atomization and consumption

   Fuel properties, both physical and chemical, including alternative fuels and sooting characteristics

6. There were two papers on unsteady flows both applied to afterburners. These were an important part of the propulsion system and would benefit from the application of modeling techniques for both steady and unsteady flows. There are other areas in combustion systems where unsteady flows may be important, e.g., the combustor inlet diffuser.

7. There are a number of other important aspects which were not directly addressed:

   Turbulence/radiation interaction

   Turbulence/droplet interaction

   Sensitivity studies including the effects of model assumptions and of boundary and initial conditions

8. Of particular importance are a series of questions relating to numerical aspects. There were no papers devoted exclusively to numerical methodologies. Questions needing attention are:

   Stability

   Grid independence

   Arbitrary curved geometries

   Accuracy

and above all computational speed. Computational speed is relevant to both the research worker in developing models and the user, applying models to problems of combustor design.

7. RECOMMENDATIONS

This meeting has demonstrated the commonality of the problems and of the approaches being adopted by the member nations of NATO in the design of advanced combustor systems. A continuing dialogue between research workers and designers will enhance the development and application of combustor models. Accordingly, it is recommended that:

1. A meeting be held in 1-2 year time for the purpose of defining a set of experiments for the further development, validation and refinement of combustor models. This meeting would serve as a focal point of the results presented at the meeting reported here and at the forthcoming PEP meeting on Measuring Techniques in Heat Transfer and Combustion (Brussels, May 1980).

2. That increased participation by industry at future meetings be encouraged.

3. That, in the call for papers, there be included a specific set of questions around which the contributed papers should be structured.

4. That the final session of the meeting be devoted to a discussion summarizing progress made towards answering the questions originally proposed.

These recommendations are intended to lead to a well coordinated and effective interchange of information.

5. In addition, the conclusions above indicate those areas where additional research work would be beneficial and are recommended.

REFERENCES – Conference Papers

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Swithenbank, J. Turan, A. Felton, P.G. Spalding, D.B.	*Fundamental Modeling of Mixing, Evaporation and Kinetics in Gas Turbine Combustors*	2	2
Jones, W.P. McGuirk, J.J.	*Mathematical Modeling of Gas Turbine Combustion Chambers*	3	4
Janicka, J. Kollmann, W.	*A Prediction Model for Turbulent Diffusion Flames Including NO-Formation*	4	5
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Elbahar, O. Wittig, S.L.K.	*On the Prediction of Temperature Profiles at the Exit of Annular Combustors*	6	7
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14. Abstract

The task of this report is to evaluate the AGARD Propulsion and Energetics Panel 54th (B) Specialists' Meeting on Combustor Modelling, which was held at DFVLR , Cologne, Germany, from 3 to 5 October 1979. After a short introduction, the meeting papers are classified into a lot of categories concerning model elements, dimensionality, survey type, application and theoretical development. The first evaluation follows this classification, while other evaluations are related to the manufacturer's and the researcher's point of view. The report is finalized with conclusions and recommendations for future treatment of combustor modelling.

The full papers of the Proceedings are published as AGARD Conference Proceedings No.275.

This Advisory Report was prepared at the request of the Propulsion and Energetics Panel of AGARD.

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