

Chapter 1: Introduction and Bibliographical Review

In this chapter the main characteristics and elements present in modern gas-turbine combustors are introduced. Next, an overview of literature related to gas-turbine combustor simulation will be presented. The main types of combustor models will be identified, with their strengths and limitations. From this review a certain type of modeling need which appears to have received little attention will be identified. The model described in this dissertation will be oriented to the satisfaction of this need.

1.1. Introduction

This section will introduce the main types of gas-turbine combustors covered in this dissertation. For a more comprehensive review of combustor types, design requirements, and historical development the reader is referred to the extensive bibliography on the subject (Lefebvre, 1993; Mellor, 1990; Hill and Peterson, 1992).

1.1.2. Straight-Flow Combustors

It is known that overall fuel/air ratios needed to achieve required temperature-rises across the combustor section of a gas turbine are too lean to sustain combustion. Therefore the established practice is to combine the fuel with only part of the total air so as to ensure the mixture is within flammability limits. The remaining air-flow is used to cool down the products of combustion to the desired exit temperature (Lefebvre, 1983).

Figure 1.1 shows a typical configuration for a straight-flow annular (axisymmetric around the engine axis) combustor. The total air flow-rate w_{inlet} coming from the compressor is divided into upper, lower, and center flow-rates w_u , w_l , w_c . The first two (between casing and liner walls) are called **annular** paths. The center path is the **primary** path. This primary flow (after passing through a dome for flame-stabilization purposes) will react with the injected fuel. Since the mixture will usually be near stoichiometric the resulting temperature will rise well above the maximum tolerable for turbine blades. Therefore cold air from the annular streams comes into the primary through bands of **dilution holes** circumferentially disposed around the liner walls. This additional air burns any remaining fuel and then cools down the products of combustion. In most cases all the an-

annular flow-rates end up in the primary, but in some instances some of the air may come out at the exits of the annular paths.

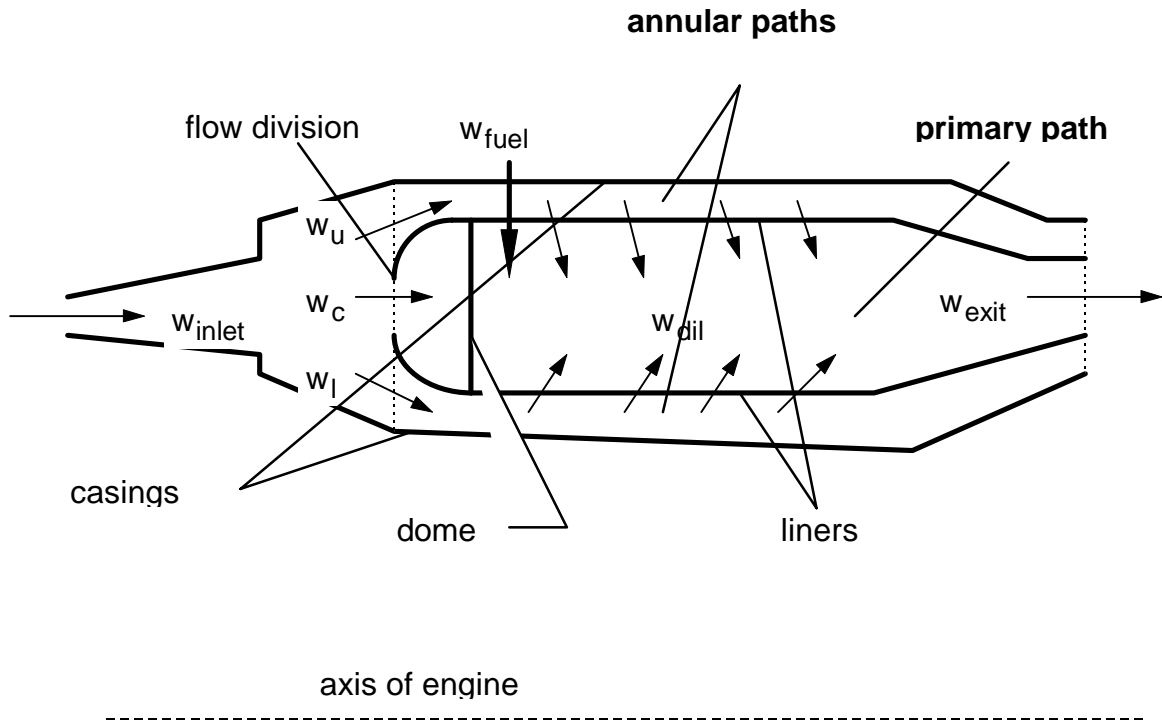


Figure 1. 1: Generic straight-flow annular combustor

1.1.2. Reverse-Flow Combustors

The previous type of combustor is usually associated with large engines. For smaller engines reverse-flow combustors are widely used, due to its efficient use of available volume (Lefebvre, 1983).

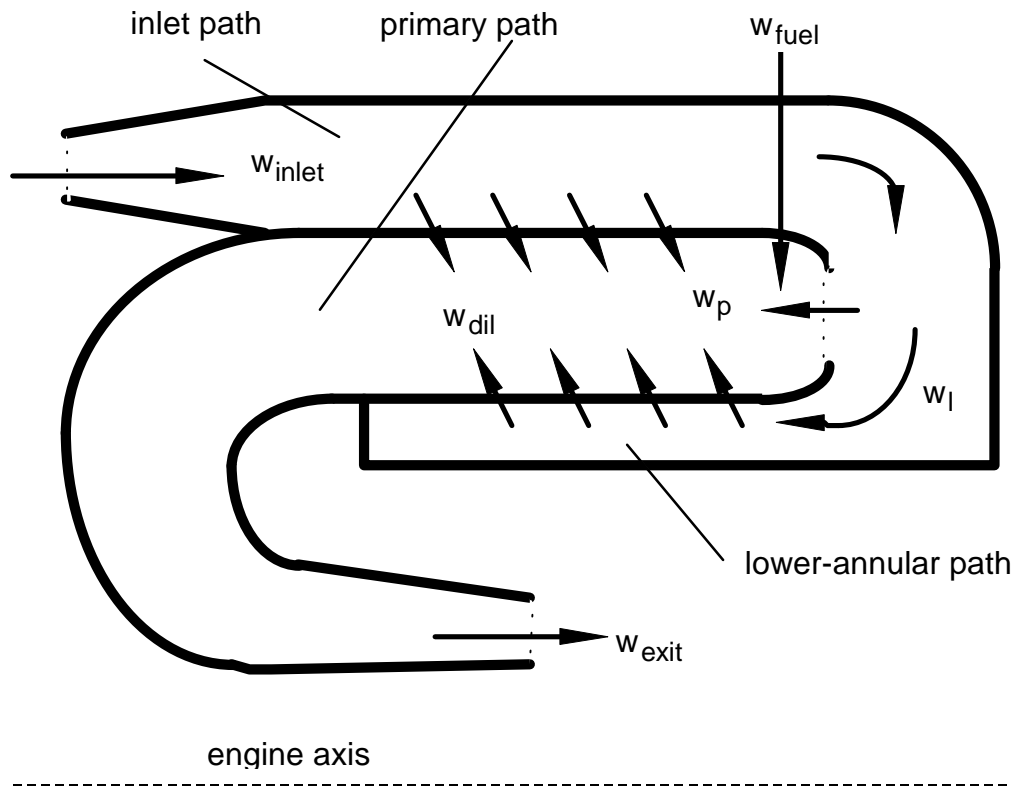


Figure 1. 2: Reverse-flow combustor configuration (open-inlet primary)

Figure 1.2 shows the main characteristics of a reverse-flow, open-inlet primary, annular combustor. The main difference with the straight-flow geometry of Fig. 1.1 is that the inlet flow-path divides in two: the primary and the lower-annular paths. Furthermore, before reaching the flow division, the inlet stream flows into

the primary through bands of dilution holes in the upper-liner wall. Since in most cases the annular exit is closed, all the air in the lower-annular path ends in the primary. As mentioned before this is an open-inlet primary type of reverse combustor. As will be shown in Chapter 3 there are examples where the inlet may be closed; in those cases all the air into the primary will come from the dilution holes.

1.2. Bibliographical Review

As soon as gas-turbine propulsion engines entered service, efforts began to develop models to simulate the entire engine and each of its components, in particular the combustion section. Needless to say these efforts were initially hampered by the physically-complex processes involved and the limitations in the existing computational hardware. As more powerful computers became available better analytical/numerical tools were developed. Zero- and one-dimensional models were soon followed by multi-dimensional ones. The following sub-section will focus on the latter type, after which we will come back to the former.

1.2.1. Full Navier-Stokes Simulation

The first multi-dimensional codes appeared in the 1970s, and aimed at the solution of the full Navier-Stokes equations including finite-rate chemistry. Among the earliest papers, some appeared in the first AGARD symposia on combustion and fuels in gas-turbines (AGARD, 1980). In subsequent meetings (AGARD 1987, 1993) improvements were made on these methods and new ones appeared. A full review of these techniques will not be attempted here. Instead the general philosophy behind these methods and their strengths and limitations will be highlighted.

The unsteady Navier-Stokes (NS) equations govern all types of turbulent flows that fall under the continuum assumption. These flows would include confined, recirculating, multiphase, reacting flows typical of gas-turbine combustors. The main problem associated with the direct solution of the NS equations is the smallness of the time and space scales of the turbulent motion compared with those of the main flow. Therefore, all practical computations solve some time-averaged form of the NS equations, also known as Reynolds equations of mo-

tion (hereafter referred to as “Reynolds equations”): each flow variable is replaced by a mean component plus a fluctuation, substituted in the original NS system and the resulting equations averaged. The Reynolds equations look very much like the NS equations, but now the unknowns are the mean values of the main variables, and additional terms are present. These additional terms represent turbulent fluxes that originate in the main flux-terms of the NS equations. To close the system these turbulent quantities have to be related to the mean main-variables by means of turbulence models. The usual practice is to model the momentum turbulent fluxes, and evaluate all other fluxes using the Reynolds analogy (Anderson et al., 1984).

The turbulence model most frequently used in combustion applications is the k - ϵ model (Schetz, 1993; Kuo, 1986). It relates the turbulent fluxes to the mean velocity gradients through a “turbulent” viscosity (Boussinesq assumption), which in turn is related to the kinetic energy of turbulence k and a turbulent dissipation rate ϵ . These two variables are obtained from the solution of transport equations derived from the original NS equations, and which are also partial differential equations. This increases the complexity of the original numerical problem, but allows the “history” of the flow to be accounted for in the turbulent viscosity.

The main problems with this model is that it is based on the Boussinesq assumption (for which there is no physical requirement that it holds), and that additional turbulent terms and constants appear in the transport equations, and which have to be modeled or specified, “... in keeping with the postulate that in turbulent flows, an equation can be derived for about anything, but none of them can be solved exactly” (Anderson et al., 1984).

Several researchers pointed some of the inadequacies of these models to capture the quantitative aspects of flows within combustors, among other reason for their dependence on constants obtained from less complex flows (Maidhof and Janicka, 1993), and because the standard k - ϵ assumes isotropic turbulence which may not be true in recirculating or swirling flows (Hwang et al., 1993). The Boussinesq assumption is frequently cast into doubt in combustion and other applications (Schetz, 1993; Correa and Shyy, 1987). In any case the need to model the additional terms and constants that appear in these and any other turbulence models means that the solution of the Reynolds equations cannot be entirely reduced to first principles, but have to be complemented by physical analogies, experience and intuition. The resulting models are not universally valid, but have to be adapted to at least different types of flows, if not to each particular case.

Independent of turbulence modeling there is the question of chemistry modeling, i.e., evaluation of the species production-rates source-terms as functions of the main variables (see Chapter 2). The almost-universal approach is to calculate these terms by means of Arrhenius forms, which are empirical expressions with some kinetic-theory foundation (Turns, 1996). These forms depend on the usual experimentally-based constants and on the reaction mechanism being postulated. This is a source of another problem: detailed mechanisms have been obtained only for a few simple fuels like methane (Westbrook and Dryer, 1981). More realistic fuels require simplified global mechanisms. This in itself is not so great an obstacle, because detailed chemistry could not be handled anyway due to prohibitive computational costs. Most common models use two- or four-step mechanisms (Turns, 1996; Frenklach, 1991). Overall formal rate equations are postulated and their rates are expressed with formal Arrhenius expressions. The parameters in the expressions are determined to fit flow-reactors and shock-tube

measurements. However, high-quality fits should not be expected for a wide variety of flows. This may have an effect in predicting, for example, temperature fields (Lee and Fricker, 1997). On the other hand, and since most gas-turbine combustors are of the non-premixed or diffusion type, a considerable number of researchers use an equilibrium or fast-chemistry model (Alizadeh and Moss, 1993; Baron et al., 1994; Di Martino et al., 1994). In this model, the species-conservation equations are replaced by the transport equation of a mixture-fraction variable; under the infinite-rate assumption the mixture fraction completely defines the composition. The approach reduces the number of equations to be solved and avoids the stiffness associated with chemical source-terms (see Chapter 2). Either with the reduced mechanism or the fast-chemistry approaches, species which are thermally insignificant but are important for other reasons (i.e., pollution) can be obtained by post-processing the numerical solution, imposing a production mechanism over the calculated flow-field (Alizadeh and Moss, 1993; Di Martino et al., 1994).

Turbulence and chemistry modeling are in reality coupled because reaction rates are highly nonlinear functions of the instantaneous values of the main variables, not just their mean values. Therefore the mean reaction-rates (that appear in the Reynolds equations) are not the reaction rates evaluated with the mean variables. One possibility is to evaluate the production rate by both an Arrhenius expression based on mean values and an eddy break-up model to account for the effects of turbulence, and use the smaller of the two (Gupta and Lilley, 1985; Kuo, 1986). This approach is based more on intuition than on first principles, but they have enjoyed some success and some argue this is due to the assumption that the combustion rate is proportional to the inverse of the turbulent time-scale (Gran et al., 1993). Another approach is the use of Probability-Density Functions (PDFs) (Khalil, 1982; Pope, 1991) They are being used in practical applications

with more frequency (Topaldi et al., 1996), usually in conjunction with the fast-chemistry model (Alizadeh and Moss, 1993; Di Martino, 1994), but in all cases it requires greater computational effort.

It is relatively common to assume that the flow is single-phase or locally homogeneous, which implies fast fuel-droplet evaporation or equivalently infinitely-small droplets. Some researches do not consider this assumption to be appropriate in practical combustor applications, and therefore take into account two-phase interaction. This means writing additional equations for the liquid phase and coupling them with the Reynolds equations for the gas phase. Two approaches are common, depending on whether the discrete particles are followed along their trajectories or the liquid phase treated as an interacting continuum: Lagrangian and Eulerian (Sirignano, 1993; Hallmann et al., 1993). Also the different methods can be classified as deterministic or stochastic, depending on whether the effects of turbulence are neglected or accounted for. Whatever approach is used the complexity of the solution procedure is considerably increased. In addition a fair amount of modelization (and uncertainty) is introduced regarding droplet-size distribution, droplet drag, heat- and mass-transfer coefficients, temperature within droplet, etc.

Another modeling issue has to do with the specification of boundary conditions. These may come from experimental data or, more frequently, from previous numerical calculations. Some researchers report solutions to be sensitive to inlet conditions, particularly when a swirler is present (Hwang et al., 1993; Danis et al., 1996). Sometimes these conditions have to be “reasonably changed” in order to “tune” the model to match available data (Lawson, 1993; Danis et al., 1996).

In brief, the impossibility of solving the NS equations with complete reaction mechanisms in a multi-phase environment requires a modeling effort for turbulence, chemistry, turbulence-chemistry interaction, two-phase interaction and specification of boundary conditions. This effort can not be reduced to first principles but requires a substantial input in the way of assumptions and empirical data, which in turn does not allow for a universal methodology. Mongia and his colleagues have acknowledged some of these issues, and have developed “hybrid” procedures by which the results of computational fluid-dynamic (CFD) calculations are fed into semi-empirical correlations to predict emission, efficiencies, temperature pattern-factors, etc. (Rizk and Mongia, 1986, 1993a). Alternatively they would “anchor” or calibrate a CFD code to a specific (baseline) combustor and then apply it to totally different designs (Danis et al., 1996), or to model the effects of design changes in the baseline combustor (Lawson, 1993). The authors report success in the use of these approaches for gas-turbine combustor design. However, they also underscore the limitation of state-of-the art combustion modeling.

As these models become more complex in an attempt to improve the accuracy of the equations in which they are based, greater demands are placed on the numerical methods needed to solve them. The vast majority of applications are based on the SIMPLE methodology introduced in the 1970s by Spalding and Patankar (Patankar, 1980; Khalil, 1982; Gupta and Lilley, 1985). It is based on the sequential solution of the governing equations together with a velocity-pressure correction. This approach offers a “simple” way to add transport equations for variables as needed. This method was among the first to be used in combustion applications, and still remains the most widely used (most papers cited so far are of this type). Other researchers complain of poor convergence

due to the sequential approach and the explicit treatment of the chemical source-terms (Chen and Shuen, 1993). Therefore they have started using strongly-coupled and fully-implicit schemes, popular in non-combustion applications (Shuen and Yoon, S., 1988; Chen and Shuen, 1993). The downside of these methods is given by their complexity and greater computer-storage requirements.

In any case it is fair to say that the numerical methods currently used are well established and are in themselves less of a source of theoretical problems as are the modeling problems previously outlined. However, it is their application which imposes restrictions. They require intensive computations per computational node, proportionally to the complexity of the different models that are adopted. Furthermore, to model realistic geometries with any degree of accuracy tens or even hundreds of thousands of nodes are needed just for the primary-flow part of the combustor. This, in turn, requires tens of hours of CPU time on current workstations, just for a single operating condition.

In brief, the modeling effort necessary to solve the Reynolds equations and the demands it places on the numerical methods imposes some limitations on their practical use:

- The impossibility to proceed “from metal to model” using exclusively first principles involve a degree of uncertainty in any practical application. This uncertainty can be used to some advantage by the modeler to “tune” the model, but necessarily restricts their universal applicability.
- The intensive computational effort required to solve the governing equations puts a definite limit on the size of the physical domain that can be solved in a

given computational run. If the solution is required for a complete configuration, it usually proceeds in two successive steps (McGuirk and Spencer, 1996). First, external flows into and around the primary flow are calculated. This may be done with CFD methods (conditions inside the primary have to be assumed) (Karki et al., 1992), or with one-dimensional codes (Lawson, 1993; Di Martino et al., 1994). Whatever method is used, all the mass flow-splits into the primary are obtained (as mentioned before, sometimes they may be obtained from experimental data). The next step is to calculate the internal flow with the previous mass-splits as inputs (no attempts are apparently made to iterate between both calculations). In other applications where more detailed information is required within the primary-flow (i.e., finer grids) a sequential multi-block approach is used in that part of the combustor (Crocker and Smith, 1993).

- Almost all of the available solutions are for steady-state conditions. Even unsteady methods are used as an efficient way to achieve steady-state. Transient simulations could be used to predict weak extinction limits (Allan, 1996) or responses to variations in air and/or fuel flow-rates. Not surprisingly, they are rarely attempted with conventional CFD methods.

CFD has become an indispensable tool in the design of modern gas-turbine combustors. Several researchers report fair to good quantitative results (Crocker and Smith, 1993; Lawson, 1993; Baron et al., 1994; Di Martino et al., 1994). As mentioned before they have been used successfully in design applications to improve existing designs (Crocker and Smith, 1993; Lawson, 1994) or to predict the performance of completely new combustors (Danis et al., 1996). The main point to be made here is that these methods just have not reached the level of accuracy and ease of use that would allow them to be the sole analytical tool.

Therefore in the design process there is still a place for lower-order methods, based on basic principles and some empirical information, that can tackle problems not currently handled by CFD solvers on a routine basis, and provide insight into the overall performance of a combustor before applying more sophisticated numerical tools or resorting to full-scale tests.

These models would be tailored to specific designs, based on the one-dimensional form of the equations, with simple chemistry models, and with limited empirical information from a given design at some specified operating conditions. These models would then be used on other conditions or even other designs. They will be considered in the following sub-section.

1.2.2. Zero- and One-Dimensional Models

Odgers (1980) distinguishes between zero- and one-dimensional models. Among the first type he includes all those models that treat the reaction zone as a single unit, such as Longwell's well-stirred reactors (Herbert, 1957). Odgers and his colleagues came with similar models calibrated to fit available experimental data (Kretschmer and Odgers, 1972, and Odgers and Carrier, 1973) The purpose of these models is usually restricted to describe blow-out phenomena and combustion efficiency.

The category of one-dimensional models includes those in which the primary-flow region is modeled by a network of stirred- and plug-flow reactors (Turns, 1996). In general the determination of the volumes and connectivity of these reactors is based on experience (Hammond and Mellor, 1973) or CFD calculations (Swithenbank et al., 1980, and Mongia, 1993b). The air inputs into the primary-flow have to be provided. The simplicity of these models allow for the use of more sophisticated chemistry models than their CFD counterparts. They have

been used with mixed success in the determination of emission and blow-out conditions.

Another approach pursued by researchers at Pratt and Whitney (Mosier et al., 1980) is to divide the primary into stream-tubes whose boundaries have to be determined. Steady-state forms of the governing equations are solved along these stream-tubes. This analysis is coupled with a multi-step chemistry model. The researchers were mainly interested in NO emissions, reporting good comparison with data.

All these analyses dealt with the primary-flow region of the combustor. As observed before all the flow-rates into this region had to be provided. Their calculation may be therefore of interest. Among the first models to attempt the calculation of flow into the primary zone was Samuel's (1961). In this model a complete annular combustor was divided into stations and the solution marched from the inlet downstream station by station. The equations solved between stations were the standard perfect-gas gas-dynamic relations. The user had to provide the flow division into annular and primary paths. Also the temperature distribution inside the primary-flow was "chosen by the designer". Among its most interesting features was the interaction between primary and annular paths through dilution holes, using incompressible orifice-theory relations. This simple model was apparently still used not long ago at General Electric (Burrus et al., 1987; Lawson, 1994).

As mentioned before some one-dimensional models are used on the exterior part of the primary flow to provide boundary conditions to CFD calculations within the primary (Lawson, 1993; Di Martino et al., 1994).

More recently Stuttaford (Stuttaford and Rubini, 1996) used a network approach to solve for complete combustor geometries. Their results compared well with a Rolls-Royce one-dimensional code.

The present author (Rodriguez and O'Brien, 1997) used a control-volume approach to model complete combustor geometries. This model was inspired by Samuel's, particularly his account for dilution holes. However, it calculated both the flow-split (with some empirical information regarding pressure-loss distribution) and the temperature in the primary flow. Also, mixed inlet and exit boundary conditions could be imposed.

So far these analyses are all steady-state. There is not much literature for unsteady calculations for gas-turbine combustors, in spite of the fact that combustor dynamics has been considered essential for post-stall behavior (Przybylko, 1985). One of the few transient models in the open literature is that of Clark and Green (1990). It is difficult to describe this model, since little information is given about what equations are being solved.

Unsteady one-dimensional models for reacting flows have been developed and used in other applications. One such example is pulse combustors. One of these models (Barr et al., 1988) uses a control-volume approach. The integral form of the governing equations are applied to the one-dimensional finite- or control-volumes in which the domain was discretized. The resulting system is solved with a MacCormack scheme (Hirsch, 1988). It should be noted that they only solve the continuity, momentum and energy equations. The heat-release due to chemical reactions, which would require the solution of species-conservation equations, is explicitly given as function of time.

To address the need for gas-turbine combustor models in post-stall engine simulations, the present author developed a very simple one-dimensional, perfect-gas, unsteady model. It has some similarities with the pulse-combustor model previously described. The complete combustor was represented by a single flow path, and the user had to provide the heat-release of the fuel. Roe's method and a Runge-Kutta procedure (Hirsch, 1988) were used to integrate the equations. Simple blow-out correlations were used for flammability limits. This model was applied to commercially-available engine simulation codes (Garrard, 1995).

1.2.3. Present Model

The model presented in this dissertation is a distant relative of the single-path model described before. As in the author's steady-state model, it accounts for flow-splits within a complete combustor configuration. The unsteady one-dimensional governing equations for reacting-flows are solved, including conservation equations for each species. This allows automatically for the heat-release within the primary flow and for finite-rate effects. It is expected that this approach can provide useful information and bridge the gap between empirically-based models and the more complete CFD simulations.