

Chapter 2

CFD Simulation of Reacting Flows

In this chapter we examine the basic ideas behind the direct numerical solution of differential equations. This approach leads to methods that can handle nonlinear equations. The simplest methods to understand are developed using numerical approximations to the derivative terms in the partial differential equation (PDE) form of the governing equations. Direct numerical solutions of the partial differential equations of fluid mechanics constitute the field of computational fluid dynamics (CFD). CFD is now on par with experiments and theory as a research tool to produce multi-scale information which can not be obtained using any other technique. There are several possible solution techniques in CFD investigation of reacting flows and a choice needs to be made for the proper technique that is to be applied in the present research.

2.1 Solution Techniques

The basic idea is to model the derivatives present in the PDEs by finite differences. When this approach is used the entire flowfield must be discretized, with the field inside the combustor defined in terms of a mesh of grid points. We need to find the flowfield values at every mesh

(or grid) point by writing down the discretized form of the governing equation at each mesh point. Discretizing the equations leads to a system of simultaneous algebraic equations. A large number of mesh points is usually required to accurately obtain the details of the flowfield, and this leads to a very large system of equations. Especially in three dimensions, this generates demanding requirements for computational resources.

When formulating a mathematical representation of a fluid flow problem, careful consideration must be given to both the flowfield model equations and the boundary conditions. An evaluation of the mathematical type of the PDEs that are being solved plays a key role in this. Boundary conditions must be properly specified. Either over- or under-specifying boundary conditions will lead to an inaccurate solution. A proper formulation requires:

- governing equations
- boundary conditions
- coordinate system specification.

If all the three conditions are satisfied, then the mathematical problem being solved is considered to be *well posed*. CFD is usually associated with computers with large memories and high processing speeds. In addition, massive data storage systems must be available to store computed results, and ways to transmit and examine the massive amounts of data associated with a computed result must be available. Before the computation of the solution is started, the mesh of grid points must be established. Thus CFD is associated with many different specialized technology areas [14]:

- grid generation
- flowfield discretization algorithms
- efficient solution of large systems of equations
- massive data storage and transmission technology methods

- computational flow visualization

Finite difference approximations of derivatives can be used to replace the individual terms in partial differential equations. Figure 2.1 provides a schematic of the steps required, and some of the key terms used to ensure that the results obtained are in fact the solution of the original partial differential equation. Successful numerical methods for partial differential equations

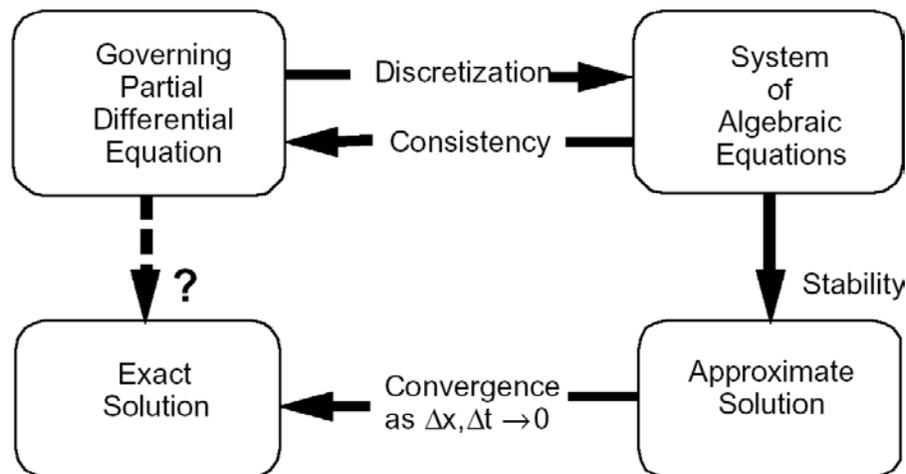


Figure 2.1: Steps and requirements to obtain a valid CFD solution

demand that the physical features of the PDE be reflected in the numerical approach. The selection of a particular finite difference approximation depends on the physics of the problem being studied. The type of the PDE is crucial, and thus a determination of the type, i.e. elliptic, hyperbolic, or parabolic is extremely important [15]. The mathematical type of the PDE must be used to construct the numerical scheme for approximating partial derivatives.

2.1.1 Finite Volume Method

Finite-difference methods are the most well known methods in CFD. However other methods have also proven successful, and one method in particular, the finite-volume technique [16], actually forms the basis for most current successful codes. In contrast to the finite difference

idea, approximations to the integral form of the governing equations result in the finite-volume approach. The other methods in use are categorized as finite element and spectral [17, 18]. Each method eventually leads to a large set of algebraic equations, just as with the finite-difference methods. In the finite-volume method, instead of discretizing the PDE, the integral form of the equations are solved. The integral form is more fundamental, not depending on continuous partial derivatives.

The results of the finite-volume approach can lead to the exact same equations to solve as the finite-difference method on a simple cartesian mesh. However, there are differences in the way the governing equations are solved in both the methods. The finite-difference method approximates the governing equation at a point whereas the finite-volume method does so over a volume. Therefore, both the finite-difference and finite-volume methods are very similar. The finite-volume method has advantages over the finite-difference method. These are:

- Conservation of mass, momentum, and energy using integrals when mesh is finite size
- Easier to treat complicated domains – integral discretization easier to implement

2.1.2 Commercial CFD Codes

In the present study, the emphasis was on applying CFD to understand the effect of acoustics on premixed flame dynamics. The idea was not to get into development of an in-house CFD code. Therefore, it was decided to use commercially available CFD codes. Although, it probably is a good idea to create a new code or develop an available code for performing fundamental studies in combustion, commercial CFD software does prove more economical in certain cases. Typical advantages of commercial CFD software include:

- Most licenses include some degree of training, which can save a great deal of time.

- Commercial software generally includes thorough documentation for understanding the usage of the code. However, most commercial software companies do not include adequate documentation on the technical details of the code. The absence of details of the code can (and does) affect the ability of the user to apply the code most efficiently and effectively.
- Commercial licenses usually include significant amounts of support, although support in the case of university licenses is rarely forthcoming. This lack of support is primarily due to the fact that university licenses cost a fraction of the amount an industrial license costs.
- Many commercial software packages combine codes developed for a variety of different applications. To the extent that such a combination is successful, this saves users who need full-spectrum capability the trouble of learning and maintaining different codes for different problems.
- Commercial software often works on a wide variety of platforms including supercomputers, parallel clusters, UNIX, and PCs. If a change in platforms is necessary, as it has been in the present study, the commercial codes are normally available for almost all popular platforms. Given the difficulty and expense of porting large codes between platforms, especially the graphical parts, commercial codes have a distinct advantage over in-house CFD codes.
- Most commercial software includes reasonably user-friendly graphical user interfaces.

Several popular commercial CFD codes are available in the market. A comprehensive list of the leading vendors can be found on the ICEM CFD website [19]. Amongst the leading vendors are **ANSYS-CFX** (*CFX: 3D fluid flow/heat transfer code*), **Fluent Inc.** (*FLUENT, FIDAP, POLYFLOW, GAMBIT*), **AeroSoft, Inc.** (*GASP, GUST, SENSE*), **NUMECA International s.a.** (*FINE, FINE/Turbo, FINE/Aero, IGG, IGG/Autogrid*), **CFD Research Corporation** (*CFD-ACE+: reacting flows*) and **CD adapco** (*STAR-CD*).

The commercial CFD software FLUENT [20] is a fully-unstructured finite-volume CFD solver for complex flows ranging from incompressible (subsonic) to mildly compressible (transonic) to highly compressible (supersonic and hypersonic) flows. The cell-based discretization approach used in FLUENT is capable of handling arbitrary convex polyhedral elements. For solution strategy, FLUENT allows a choice of two numerical methods, either segregated or coupled. With either method FLUENT solves the governing integral equations for conservation of mass, momentum, energy and other scalars such as turbulence and chemical species. Both segregated and coupled numerical methods employ a similar finite-volume discretization process but their approach to linearization and solution of the discretized equations is different. A point implicit (Gauss-Seidel) linear equation solver is used in conjunction with an Algebraic Multigrid (AMG) scheme to solve the resultant linear system for the dependent variables in each cell. In the present study, laminar flame dynamics has been investigated by applying the FLUENT solvers.

For the turbulent flame dynamics part of the study, both FLUENT and CFD-ACE+ have been applied. CFD-ACE+ is a general, partial differential equation (PDE) solver for broad range of physics disciplines including: flow, heat transfer, stress/deformation, chemical kinetics, electrochemistry etc.

2.2 Reacting Flow Simulation

The term ‘reacting flows’ applies to a broad range of physical phenomena. For gas-phase reacting flows, a set of time-dependent, coupled PDEs governs the conservation of mass, momentum, species density and energy. The PDEs describe the motion of the fluid, species reactions, transport processes like conduction of heat, molecular diffusion and thermal radiation. Oran and Boris [21] describe the set of PDEs needed to be solved for reacting flow simulation and describe the various physical processes that change the species densities and transport energy. These processes are:

Convection is a continuum concept, which assumes that quantities such as density, velocity and energy are smoothly varying functions of position. Convective effects are represented in the PDEs by fluxes of conserved quantities ($\nabla \cdot \vec{v}\phi$, where ϕ is ρ , $\rho\vec{v}$, E etc.)

Chemical reactions amongst species are represented by the production and loss terms in the energy equation. The species conservation equations are solved separately to calculate the production and loss terms.

Diffusion effects are represented as a divergence of a flux. Changes in energy due to molecular diffusion and chemical reactions are accounted for in the heat flux.

Radiation transport is represented in the energy equation as a source term, in effect decoupling the complexities of radiation modeling from the conservation equations.

Wave phenomena is described in the reacting flow conservation equations by coupled sets of continuity equations.

The first four processes are all identified with specific terms in the reacting flow conservation equations set. Wave phenomena on the other hand happens because of the interaction between distinct terms in the Navier-Stokes equations. Energy in the medium can be moved by waves to another location where the composition of the medium may be different. The inertia term ($\partial\rho\vec{v}/\partial t$) in the momentum equation is a key parameter of wave phenomena. The inertia causes a time delay between the application of a force and the response of the medium to that force. This time delay determines the frequency and the effective speed of propagation of the wave. The existence of a characteristic frequency can allow resonances when a small input of energy over time (in the correct phase with the wave) can lead to very large amplitudes of pressure fluctuation.

Chemical reactions are generally considered in terms of unimolecular or bimolecular reactions amongst interacting species. A set of non-linear, first-order, ordinary differential equations describe rate of changes due to interactions among species. No spatial gradients or derivatives

are present in these equations. The expressions for the rates commonly encountered in combustion kinetics are usually written in an *Arrhenius form*:

$$AT^b e^{-c/T} \quad (2.1)$$

Temperature is calculated from the energy equation along with the Arrhenius equation for chemical kinetics. When the chemical reactions release or absorb a great deal of energy, the reaction kinetics are strongly coupled to convection through pressure and density. These highly endothermic or exothermic reactions create a strong coupling between chemistry and fluid dynamics.

2.2.1 Combustion Chemistry Modeling

In reacting flow simulation, solution of the chemical kinetics is often the most expensive part of the calculation. The smallest mechanism encountered in combustion chemistry modeling describes the oxidation of hydrogen. Nine species and approximately fifty reactions are involved in this mechanism. This number dramatically increases for higher hydrocarbons and is enormous for soot formation. For soot formation in CH_4-O_2 system, hundreds of species are present and tens of thousands of reactions are involved. Thus, integrating the chemical kinetics equations will take an order of magnitude longer than solving the convective and diffusive transport terms. The computational cost is directly proportional to the number of species, the number of reactions and the number of grid points in the domain. Since Arrhenius kinetics is a non-linear formulation, the computations become more expensive. Different approaches, therefore, are followed to reduce the computational expenses related to chemical kinetics. These approaches can be categorized in terms of methods:

- that fit data or parameters from detailed chemical mechanisms into a given form or a table,
- that use analytical techniques to derive simplified sets of reaction-like equations for a particular mechanisms, and

- that modify the mechanisms by introducing partial equilibrium or steady-state concepts.

2.3 Turbulent Combustion Modeling

Lately, much work has been devoted to modeling turbulent combustion using CFD with a variety of approaches and modeling techniques. A wide range of coupled problems are encountered in turbulent flames:

- Heat transfer, molecular diffusion, convection, turbulent transport and other such transfer phenomena that occur in turbulent flames need to be carefully described along with describing the mixing between reactants. For accurate modeling of all the above mentioned phenomena, the fluid mechanical properties of the combustion system must be well understood.
- To predict ignition, stabilization or extinction of the reaction zones and pollutant formation, precise knowledge of the chemistry involved is required. Therefore, detailed chemical reaction schemes are necessary to estimate the consumption rate of the fuel, the formation of combustion products and pollutant species.

Turbulent combustion modeling is a broad subject area and therefore it is not possible to review all possible aspects of turbulent combustion modeling in this study. The focus of this section is to introduce closure schemes that are used to understand and calculate turbulent transport and mean burning rates in turbulent flames.

The following steps (decomposition shown in Figure 2.2) ought to be followed in numerical modeling of turbulent combustion:

- Asymptotic analysis, limited to simplified situations (usually restricted to laminar combustion regime), leads to analytical results producing scaling factors like dimensionless

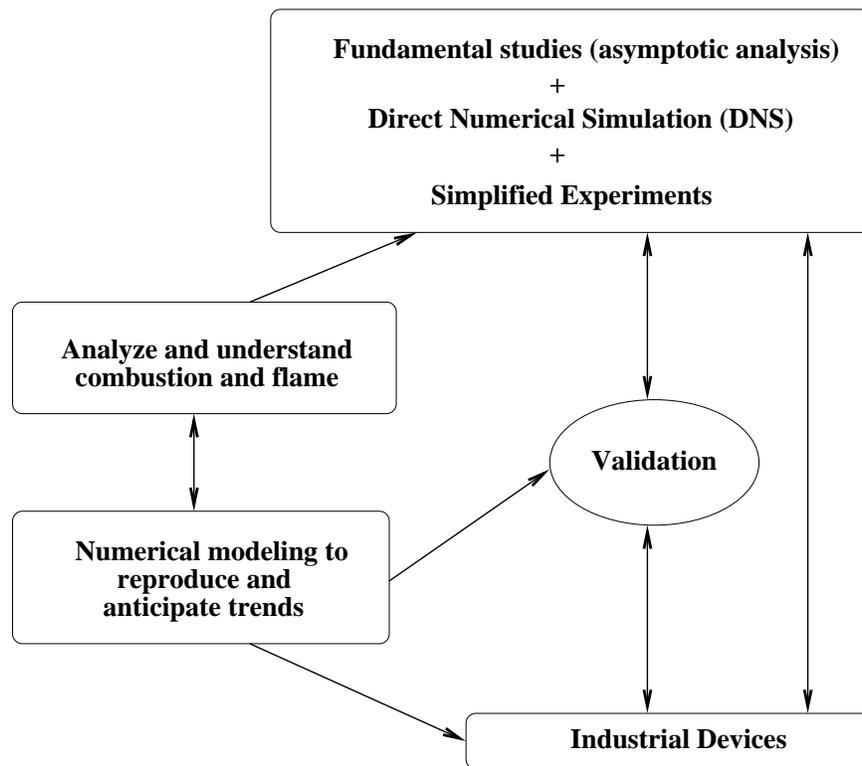


Figure 2.2: Turbulent combustion modeling steps

numbers which describe major flame behaviors.

- Experiments performed help understand the basic properties of combustion. The experiments are to be accompanied by numerical simulations of laminar flames incorporating chemistry modeling and multi-species transports along with radiative heat losses modeling.
- Direct numerical simulation (DNS) is to be performed to calculate all the scales (time and length) of turbulence without resorting to closures of turbulent fluxes and mean burning rate. The simulation is done for simple configurations to extract data which are impossible to measure in experiments.

Large number of degrees of freedom involved in turbulent combustion make a full DNS of a practical system prohibitively expensive and averaging techniques leading to unclosed equa-

tions then become necessary. The following steps are then to be followed toward modeling of turbulent combustion:

- Closure techniques are to be found in exact averaged balance equations.
- Once the models have been implemented in the code, validation against measurements from experiments are to be performed. Configurations as close as possible to actual industrial systems are to be chosen for the tests.
- The last step is the simulation of a real combustion device.

The decomposition shown in Figure 2.2 is a formal description of the modeling process. Turbulent combustion modeling efforts are usually a continuous process which includes theoretical studies in analysis of combustion, understanding flames and improving models, implementation of the models into CFD, experimental measurements and comparison between experimental data and numerical results. Full numerical solution of instantaneous balance equations (classical Navier-Stokes, species and energy transport equations) is limited to very simplified cases [22, 23], where there are not too many time and length scales present in the flow. To overcome this difficulty, an additional step is introduced by averaging the balance equations to describe only the mean flow field (local fluctuations and turbulent structures are integrated in mean quantities and these structures have no longer to be described in the simulation). Each quantity Q is split into a mean component \overline{Q} and a fluctuating component Q' :

$$Q = \overline{Q} + Q' \quad (2.2)$$

with $\overline{Q'} = 0$. Next, the instantaneous balance equations are to be ensemble averaged to derive transport equations for the mean quantity \overline{Q} . This classical Reynolds averaging technique introduces unclosed correlations such as $\overline{u'Q'}$ that are unknown and must be modeled. This numerical procedure is called Reynolds Averaged Navier-Stokes (RANS) modeling. In turbulent flames, fluctuations of density are observed because of the thermal

heat release, and Reynolds averaging induces some additional difficulties. Averaging the mass balance equation leads to:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} u_i + \overline{\rho' u_i'}) = 0 \quad (2.3)$$

where the velocity/density fluctuations correlation $\overline{\rho' u_i'}$ appears. To avoid the explicit modeling of such correlations, a Favre (mass weighted) average [24] \tilde{Q} is introduced and any quantity is then decomposed into $Q = \tilde{Q} + Q''$:

$$\tilde{Q} = \frac{\overline{\rho Q}}{\bar{\rho}}; \quad \tilde{Q}'' = \frac{\overline{\rho(Q - \tilde{Q})}}{\bar{\rho}} = 0 \quad (2.4)$$

2.3.1 Favre Averaged Balance Equations

The objective of turbulent combustion modeling is to propose closures for the unknown quantities in the averaged balance equations, such as:

- *Reynolds stresses* $\widetilde{u_i'' u_j''}$. The turbulence model provides an approximation for this term. The closure may be done directly or by deriving balance equations for these Reynolds stresses
- *Species* $(\widetilde{u_j'' Y_k''})$ *and temperature* $(\widetilde{u_j'' T})$ *turbulent fluxes*. These fluxes are usually closed using a gradient transport hypothesis:

$$\bar{\rho} \widetilde{u_j'' Y_k''} = -\frac{\mu_t}{Sc_{kt}} \frac{\partial \tilde{Y}_k}{\partial x_j} \quad (2.5)$$

where μ_t is the turbulent viscosity, estimated from the turbulence model, and Sc_{kt} is the turbulent Schmidt number for the species k . For some premixed turbulent flames this assumption may be wrong [25] when counter-gradient turbulent transport may be observed.

- *Laminar diffusive fluxes* are usually small compared to turbulent transport, assuming a sufficiently large turbulence level (large Re).

- *Species chemical reaction rate* $\overline{\dot{\omega}_k}$. Turbulent combustion modeling generally focuses on the closure of these mean burning rates.

The balance equations, closed with appropriate models, allow only for the determination of mean quantities, that may differ from instantaneous ones. Strong unsteady mixing effects, resulting from the rolling up of shear layers, are observed in turbulent flames, and the knowledge of steady statistical means is not always sufficient to describe turbulent combustion. An alternative is to use large eddy simulation (LES).

2.3.2 Filtering and Large Eddy Simulation

The objective of Large Eddy Simulation (LES) is to explicitly compute the largest structures of the flow, typically the structures which are larger than the computational mesh size, while the effects of the smaller ones are modeled. LES is widely used in context of non-reacting flows [26, 27], its application to combustion modeling is still at an early stage. As in RANS, the complex coupling between micromixing and chemical reactions occurring at unresolved scales needs models, some of which can be addressed using LES:

- Large structures in turbulent flows generally depend on the geometry of the system. On the contrary, smaller scales feature more isotropic properties. Accordingly, turbulence models may be more efficiently applied to modeling the smallest structures.
- Turbulence mixing controls most of the global flame properties. In LES, unsteady large scale mixing between fresh and burnt gases in premixed flames is simulated instead of being averaged.
- Most reacting flows exhibit large scale coherent structures [7], which are also observed when combustion instabilities occur. LES may be a powerful tool to predict the occurrence of such instabilities [28] and help improve active control systems

- LES computes the large structures explicitly as well as clearly identifies instantaneous fresh and burnt gases zones which have different turbulence characteristics.

In LES, the relevant quantities Q are filtered in the spectral space – components greater than a cut-off frequency are suppressed, or in the physical space – weighted averaging in a given volume. The filtered operation is defined by:

$$\bar{Q}(\mathbf{x}) = \int Q(\mathbf{x}^*)F(\mathbf{x} - \mathbf{x}^*)d\mathbf{x}^* \quad (2.6)$$

where F is the LES filter. Standard filters are described in [29]

Filtering the instantaneous balance equations leads to equations similar to the Reynolds averaged balance equations (RANS):

- mass:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0 \quad (2.7)$$

- momentum (for $i = 1, 2, 3$):

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = -\frac{\partial}{\partial x_j} [\bar{\rho} (\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j)] - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \bar{F}_i \quad (2.8)$$

- Chemical species (N species, $k = 1, \dots, N$):

$$\frac{\partial \bar{\rho} \tilde{Y}_j}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{Y}_k}{\partial x_j} = -\frac{\partial}{\partial x_j} [\bar{\rho} (\widetilde{u_j Y_k} - \tilde{u}_j \tilde{Y}_k)] + \bar{\omega}_k \quad (2.9)$$

- Total enthalpy ($h_t = h + u_i u_i / 2$):

$$\frac{\partial \bar{\rho} \tilde{h}_t}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{h}_t}{\partial x_j} = -\frac{\partial}{\partial x_j} [\bar{\rho} (\widetilde{u_j h_t} - \tilde{u}_j \tilde{h}_t)] + \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{J}_j^h + \overline{u_i \tau_{ij}}) + \overline{u_j F_j} \quad (2.10)$$

where \bar{Q} and \tilde{Q} denote LES filtered quantities instead of ensemble means. The unknown quantities in the equations are:

- Unresolved Reynolds stresses ($\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$), which require a subgrid scale turbulence model.

- Unresolved species fluxes $(\widetilde{u_j Y_k} - \widetilde{u_j} \widetilde{Y_k})$ and enthalpy fluxes $(\widetilde{u_j h_t} - \widetilde{u_j} \widetilde{h_t})$.
- Filtered laminar diffusion fluxes $\overline{j_j^h}$.
- Filtered chemical reaction rate $\overline{\omega_k}$.

These filtered equations, coupled to subgrid scale models are to be numerically solved to simulate the unsteady behavior of the filtered fields. Compared to direct numerical simulations (DNS), part of the information contained in the unresolved scales is lost and consequently has to be modeled. Compared to RANS, LES provides better information on the large resolved motions.

2.3.3 Regimes of Turbulent Combustion

Mean burning rate being a highly non-linear variable, it cannot be found from an averaging of Arrhenius laws because it is very difficult to express $\overline{\omega_k}$ as a function of the mean mass fractions $\widetilde{Y_F}$ and $\widetilde{Y_O}$, the mean density $\overline{\rho}$ and the mean temperature \widetilde{T} . A physical approach is required to derive models for turbulent combustion. The physical analysis is based on comparison of the various scales present in turbulent combustion. The Damkohler number compares the turbulent (τ_t) and the chemical (τ_c) time scales:

$$Da = \frac{\tau_t}{\tau_c} \quad (2.11)$$

For large values of Damkohler number ($Da \gg 1$), the flame front is thin and its inner structure is not affected by turbulence motions which only wrinkle the flame surface. This *flamelet regime* occurs when the smallest turbulence scales (Kolmogorov scales) have a turbulent time τ_t larger than τ_c meaning turbulent motions are too slow to affect the flame structure. The transition is described in terms of the Karlovitz number Ka :

$$Ka = \frac{\tau_c}{\tau_t} \quad (2.12)$$

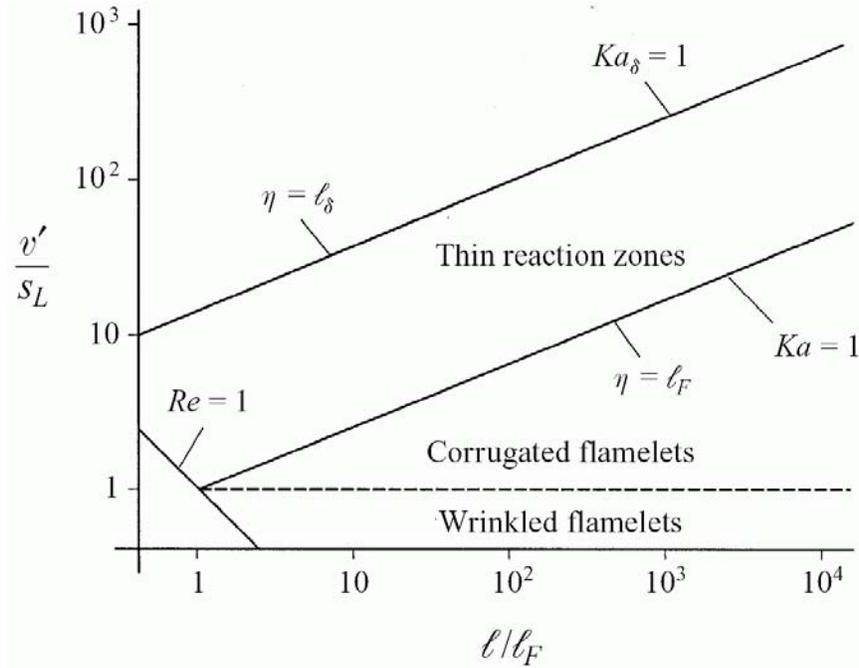


Figure 2.3: Regime diagram for premixed turbulent combustion: v' is the RMS velocity, S_L is the laminar flame speed, l is the integral length scale and l_F is the flame thickness

The Karlovitz number is used to define the *Klimov-Williams criterion*, corresponding to $Ka = 1$, delineating between two combustion regimes. This criterion differentiates between the *flamelet regime* ($Ka < 1$) and the *distributed combustion regime*. For Karlovitz numbers larger than unity ($Ka > 1$), turbulent motions are able to affect the flame inner structure but not necessarily the reaction zone. Therefore, another number, the Karlovitz number based on the thickness of the reaction zone is defined:

$$Ka_\delta \approx \frac{Ka}{100} \quad (2.13)$$

On the basis of the Karlovitz number, the following turbulent premixed flame regimes are proposed [30] (see Figure 2.3):

- $Ka < 1$: *Flamelet regime* or *thin wrinkled flame regime* (see Figure 2.4a). Two subdi-

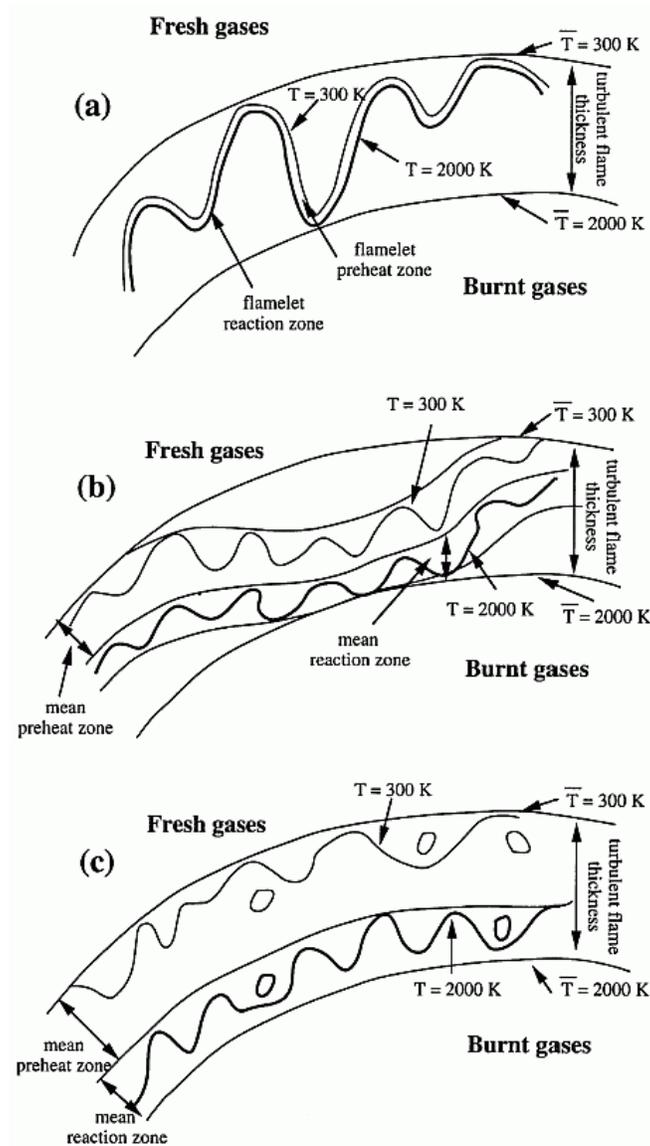


Figure 2.4: Premixed turbulent combustion regimes: (a) flamelet (thin wrinkled flame), (b) thick wrinkled flame, and (c) thickened flame

visions may be proposed depending on the velocity ratio (u'/S_L):

- $u'/S_L < 1$: *wrinkled flame*. As u' can be viewed as the rotation speed of the larger turbulent motions, turbulent structures are unable to wrinkle the flame surface up to flame front interactions. The laminar propagation is dominant and

turbulence/combustion interactions remain limited.

- $u'/S_L > 1$: *wrinkled flame with pockets/corrugated flames*. Larger structures are able to induce flame front interactions leading to pockets where such a phenomenon occurs.
- $1 < Ka \leq 100$ ($Ka_\delta < 1$): *Thickened wrinkled flame regime* or *thin reaction zone* (see Figure 2.4b). Turbulent motions are able to affect and thicken the flame preheat zone, but cannot modify the reaction zone which remains thin and close to a laminar reaction zone.
- $Ka > 100$ ($Ka_\delta > 1$): *Thickened flame regime* or *well-stirred reactor* (see Figure 2.4c). Preheat and reaction zones are strongly affected by turbulent motions and no laminar flame structure may be identified.

2.3.4 Turbulence-Chemistry Interaction Modeling

The mean heat release rate is one of the main quantities of practical interest that is to be approximated by turbulent combustion models. On the basis of the regimes of turbulent premixed combustion shown above, tools are designed to describe turbulent flames which will provide an estimation of mean production or consumption rates of chemical species. In premixed flames, predictions of radicals and intermediate species such as OH , or pollutants like CO , require the description of the flame front internal structure, for intermediate states between fresh and burnt gases. Three approaches, illustrated in Figure 2.5, which can be implemented for analyzing turbulent flames are summarized below:

- The burning rate may be quantified in terms of *turbulent mixing*. When Damkohler number is large, the reaction rate is limited by turbulent mixing, described in terms of scalar dissipation rates. The small scale dissipation rate of species controls the mixing of the reactants and plays a dominant role in combustion modeling.

- *Geometrical analysis* describes the flame as a geometrical surface and this approach is linked to a flamelet assumption (the flame is thin compared to all flow scales). In this approach, scalar fields, like the reaction progress variable c , are studied in terms of dynamics and physical properties of isovalue surfaces defined as flame surfaces (iso- c). The flame is considered to be an interface between fresh and burnt gases for premixed combustion cases. A flame normal analysis is carried out by studying the structure of the reacting flow along the normal to the flame surface.
- *Statistical properties* of scalar fields may be collected and analyzed for any location within the flow. Mean values and correlations are then extracted by using one-point probability density functions (PDF).

Probability Density Function Approach

The probability density function (PDF) method focuses on the statistical properties of intermediate states within the flame front. The probability density function $\bar{P}(Y^*; \underline{x}, t)$ quantifies the probability to find, for a given location \underline{x} and a time t , a variable Y (mass fraction, temperature, velocity, etc.) within the range $[Y^* - \Delta Y/2, Y^* + \Delta Y/2]$. This probability is equal to $\bar{P}(Y^*; \underline{x}, t) \Delta Y$ [31]. The PDF satisfies the following relations:

$$\int_Y \bar{P}(Y^*; \underline{x}, t) dY^* = 1 \quad (2.14)$$

$$\int_Y \bar{P}(Y^*; \underline{x}, t) dY^* = \bar{Y}(\underline{x}, t) \quad (2.15)$$

$$\int_Y (Y^* - \bar{Y})^2 \bar{P}(Y^*; \underline{x}, t) dY^* = \overline{Y'^2}(\underline{x}, t) \quad (2.16)$$

where Y^* is the sample space variable corresponding to the random variable Y . When more than one variable is required to capture the flame structure, a joint PDF, $\bar{P}(Y_1^*, \dots, Y_N^*; \underline{x}, t)$ is introduced. The mean burning rate is then estimated as:

$$\bar{\omega}_{Y_1}(\underline{x}, t) = \int_{Y_1} \cdots \int_{Y_N} \omega_{Y_1}(Y_1^*, \dots, Y_N^*) \bar{P}(Y_1^*, \dots, Y_N^*; \underline{x}, t) dY_1^* \dots dY_N^* \quad (2.17)$$

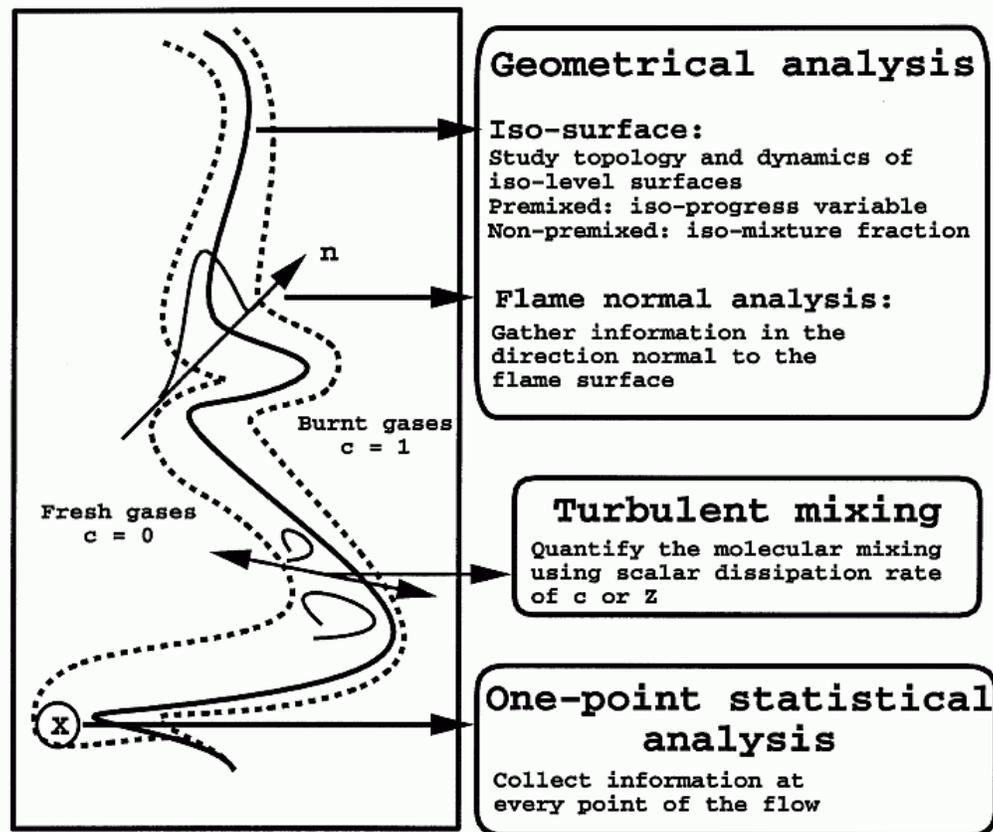


Figure 2.5: Three types of analyses for premixed turbulent flame modeling

The mean burning rate calculated using the PDF is used as a source term in the energy equation. An alternate method of estimating the mean burning rate is the use of concentration of radicals from detailed chemical mechanisms. This type of estimation, using different species mass fractions, has been followed in the turbulent combustion modeling part of the present study.