Chapter 2

Concepts and Definitions

The phenomenon of combustion dynamics involves several dynamic processes including acoustics, fluid dynamics, combustion, and heat transfer and requires a multi-disciplinary effort to analyze it, and to develop control methodologies to prevent unwanted instabilities such as thermo-acoustic instability from occurring. This documentation attempts to provide a better understanding of the combustion dynamics from both the physical and systems theory perspective. Therefore, to aid in better understanding the research work presented here, this chapter shall discuss and define the relevant terms and concepts. The following material is not intended as a complete review of the reacting flow and the systems theory, but only as a partial list of definitions and concepts, which shall be referred to throughout this work. The reader is referred to [8, 9, 10, 11, 12] for detailed discussion of combustion, and [13, 14] for discussions on systems theory and linear controls.

2.1 Combustion Terminology

2.1.1 Stoichiometric Reaction

Stoichiometric reaction is a unique reaction in which all the reactants are consumed. This means that the amount of oxidant present in the reaction is just enough to completely burn the fuel. Assuming that air consists of 21% oxygen and 79% nitrogen by volume, the equation for a stoichiometric reaction of an air-methane mixture on a mole basis is

$$CH_4 + 2(O_2 + 3.76N_2) \Rightarrow CO_2 + 2H_2O + 7.52N_2 \tag{2.1}$$

2.1.2 Equivalence Ratio

The fuel/oxidant ratio is one of the most important parameters for combustion analysis and is normally reported in terms of a non dimensional variable called equivalence ratio Φ, which is the actual fuel/oxidant ratio normalized by the stoichiometric fuel/oxidant ratio:

$$\Phi = \frac{(Fuel/Oxidant)_{actual}}{(Fuel/Oxidant)_{stoichiometric}} \tag{2.2}$$

$\Phi = 1.0$ is defined as stoichiometric condition. Conditions where there is an excess of oxidant present in the mixture are "lean", $\Phi < 1.0$. Similarly, mixtures with an excess of fuel are "rich", $\Phi > 1.0$. Equation 2.2 is valid when the ratio is calculated on both mass and mole basis, provided that the actual and stoichiometric ratios are calculated consistently.

The equivalence ratio may also be defined as

$$\Phi = \frac{(Oxidant/Fuel)_{actual}}{(Oxidant/Fuel)_{stoichiometric}} \tag{2.3}$$

For this definition, the mixture is considered to be 'lean' when $\Phi > 1.0$, while 'rich' mixtures have a $\Phi < 1.0$. This nomenclature is generally used in European literature.

2.1.3 Flame Temperature

Another important combustion parameter is the flame temperature. The flame temperature (T_f) is determined by the energy balance between the reactants and the products at equilibrium. If the reaction zone is spatially very thin in comparison to the rest of the domain of interest, then it is a common practice to denote the maximum temperature in the reaction zone to be the flame temperature. If the combustion process takes place adiabatically, and with no work, or changes in the kinetic or potential energy, then the flame temperature is

Table 2.1: Flammability limits and flame properties for some common gases at atmospheric pressure. The flammability limits apply to upward propagation in tubes. The flame temperature refers to stoichiometric mixtures, except those marked * which are maximum values [9]

Reactants	Flammability limits (% by volume)		Adiabatic flame temperature (Kelvin)	Maximum burning Velocity (meters/sec)
	Lower	Upper		
$H_2 + O_2$	4.0	94	3083	11.0
$CO + O_2 (+H_2O)$	15.5	94	2973	1.08
$CH_4 + O_2$			3010	4.5
$C_2H_2 + O_2$			3431	11.4
$H_2 + air$	4.0	75	2380	3.1
$CO + air$	12.5	74	2400	0.45
$CH_4 + air$	5.3	15	2222	0.45
$C_2H_2 + air$	2.5	80	2513	1.58
$C_2H_4 + air$	3.1	32	2375	0.75
$C_2H_6 + air$	3.1	15	2244*	0.40
$C_2H_8 + air$	2.2	9.5	2250*	0.43
n-$C_4H_{10} + air$	1.9	8.5	2256*	0.38
$C_6H_6 + air$	1.5	7.5	2365*	0.41
$C_2H_3OH + air$	3.0	80	2411*	1.05

referred to as the adiabatic flame temperature (T_{af}). This is the maximum temperature that can be achieved for the given reactants because any heat transfer from the reaction zone and any incomplete combustion would tend to lower the temperature of the products. Experimental measurements of T_{af} are very difficult and in most cases a calculated value is more reliable than the experimental measurements [9]. For most hydrocarbons, the maximum adiabatic flame temperature occurs at slightly above stoichiometric conditions ($\Phi \simeq 1.05$). However, there are exceptions to the norm such as C_2H_2. The calculated values of T_{af} for several common combustible mixtures is listed in Table 2.1.

According to "Laminar flame theory" T_f has a substantial effect on the flame speed. It is widely perceived that T_f essentially determines the flame speed and significantly influences the formations of the products of combustion. The concentration of oxides of nitrogen (NO_x) and CO, pollutants of great concern are very much dependent on T_f. More detailed information on the effect of T_f on the production of pollutants is described in [8, 9, 10, 11]

2.1.4 Classification of Flames

Flames can be classified in various ways. Based upon how the fuel and oxidizer reach the reaction front, there are non-premixed flames and partially and fully premixed flames. The nature of the reaction zone is used to categorize flames as well stirred reactors or plug flow reactors. The flow characteristics of the incoming reactants divide flame types into turbulent and laminar flames. There are a number of such flame classifications and a discussion of all of them is beyond the scope of this document. Only the relevant categories are defined and discussed below.

Non-premixed Flames

In non-premixed flames, the fuel and oxidizer are present on either side of the reaction zone. They are brought to the reaction zone in an unmixed state primarily due to diffusion of reactants into, and products out of the reaction zone. In such flames the reaction zone is established at a location where the total enthalpy of the reactants present balance the total enthalpy of the products generated plus any energy losses. Thus, for non-premixed flames the reaction ideally takes place at stoichiometric conditions, thereby producing the maximum possible flame temperature for a given combination of reactant species.

Fully Premixed Flames

In fully premixed flames, the fuel and the oxidizer are thoroughly mixed prior to reaching the reaction zone, also known as the flame front. In these flames the position of the reaction zone is not defined by the diffusion of reactants, but by balancing the local convective velocity of the reactants with the rate of consumption of the reactants popularly known as the flame speed, which is formally defined in Section 2.1.5. Based on the stabilizing method, fully premixed flames can be burned at equivalence ratios other than 1. Thus, lower flame temperatures can be achieved.

Partially Premixed Flames

In partially premixed flames, the fuel is injected into the oxidizer flow just upstream of the flame. Under such conditions, there is not enough time for the fuel and the oxidizer to mix thoroughly and thus, concentration gradients across the flow are generated in the reactant stream which enters the flame front. These flames are neither purely non-premixed, nor are fully premixed, hence they are termed as partially premixed. Such flames are characterized by their degree of unmixedness, which is a measure of how much the radial concentration profiles of the flow deviate from a fully premixed case.

Well Stirred Reactor

Well stirred reactor is an idealistic situation that can often be applied to flows with high turbulent intensities. It is a condition where the products of combustion get mixed with the reactants so quickly that ideally no temperature or species gradients remain with the reaction zone, which now has a finite volume. Well stirred reactor approximation is applied to conditions where there is tremendous mixing and reaction rates are very high

Plug Flow Reactors

When reacting flows have no mixing in the direction of flow, the combustion process is termed as plug flow reactors. Here the reactions are carried on along the flow. Thermal and species gradients are generated in the axis of the flow purely due to the diffusion process. Plug flow reactors characterize systems with no re-circulation of products and slow reaction rates.

Excess Enthalpy Flames

Pre-heating of the reactant mixture has a profound effect on the combustion rates, flammability limits, and emissions. One of the common methods to preheat the reactants is to use a

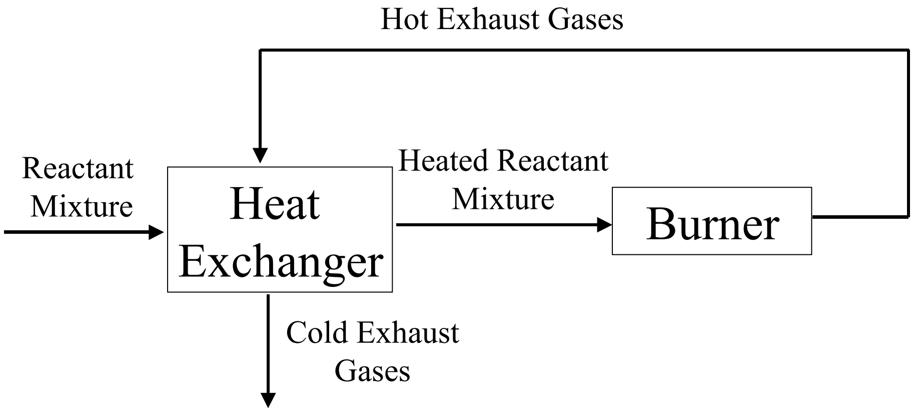

Figure 2.1: Schematic of a burner using external heat re-circulation

heat exchanger to re-circulate the energy of the exhaust gases. A schematic of such a burner is shown in Figure 2.1. This utilization of the energy of the exhaust gases to increase the inlet temperature of the reactants is often referred to as excess enthalpy burning. By the simple use of the first and second law analysis, Hardesty and Weinberg [15] showed that excess enthalpy flames are not only feasible, but are able to burn low grade fuels, reduce pollutant emissions, and increase combustion efficiency. They performed several experiments with an uninsulated fused silica burner and were able to verify their predictions to a limited extent. They concluded that by reducing the heat loss from the reaction zone, the performance of the burner could be enhanced. Modern burners use the concept of excess enthalpy flames by pre-heating the incoming reactants via the flame stabilizer, thus doing away with the problems associated with external heat exchangers

2.1.5 Flame Speed

The flame speed is defined as the local velocity of the reactant mixture normal to the reaction zone, just as the gases move into the reaction zone. As stated previously, the flame speed is essentially determined by the value of T_f. Therefore, the variation of the flame speed at adiabatic conditions (S_L) due to changes in Φ is primarily determined by the variation of adiabatic flame temperature(T_{af})[8]. The maximum value of S_L for several common fuels is listed in Table 2.1. Kuo [8] and Williams [11]discuss several methods which are currently used to experimentally determine S_L. These methods can be quite complex and accurate experimental values are difficult to obtain.

2.1.6 Flashback and Blowoff

In premixed flames, there are situations when the supply velocity of the reactant, just prior to the flame front is not sufficient to oppose the flame speed. Under such conditions, the flame propagates upstream into the incoming reactants. This is known as flashback. On the other extreme, there are conditions where the local supply velocity of the reactant is greater than the flame speed. Under such situations the flame moves downstream, a phenomenon termed as blow off.

2.1.7 Chemiluminescence

Chemiluminescence is defined as the radiation emitted by an excited molecule that enables the molecule to return to ground state. Every radiating molecule emits energy at a characteristic wavelength, which depends upon the structure of the molecule and the transition process that the molecule undergoes. This phenomenon is well explained using the laws of quantum mechanics, and its basics are discussed here.

A radiating gas can be composed of molecules, atoms, ions and free electrons. These particles can have various energy levels associated with them. A schematic diagram of the energy levels for a particle is shown in Figure 2.2. The zero level is assigned to the ground state, with higher bound states being at positive energy levels. E_I is the ionization potential that is the energy required to produce ionization from the ground state.

From the quantum mechanics point of view, a photon is the basic unit of radiative energy.

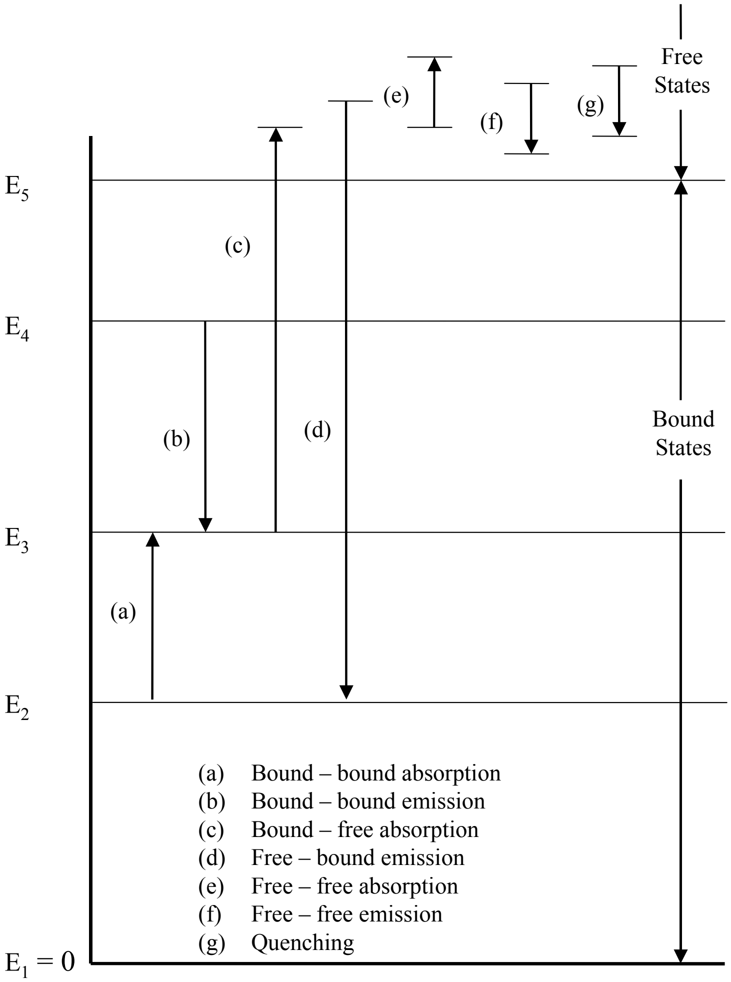

Figure 2.2: Schematic of the energy levels and associated radiation processes

Radiative emission is the release of photons of energy, and absorption is the capture of photons by a particle. Whenever a photon is emitted or absorbed, the energy of the emitting and absorbing particle is correspondingly decreased or increased. The magnitude of energy transition is related to the frequency of the emitted or absorbed radiation. The energy of the photon is $h\nu$, where h is Plancks constant and ν is the frequency of the photon energy. Thus, for energy transition from state E_2 to state E_1 a photon is emitted with energy given by

$$E_2 - E_1 = h\,\nu \tag{2.4}$$

The frequency of the emitted energy is

$$\nu = \frac{E_2 - E_1}{h} \tag{2.5}$$

Conversely only when a photon of frequency ν, given by equation 2.5, strikes a particle and is absorbed, does a particle move from E_1 to E_2. When a photon is absorbed or emitted by a particle with no ionization or recombination of ions and electrons, the process is termed bound-bound absorption or emission (process a,b Figure 2.2). Process c, in Figure 2.2 is a bound-free absorption (photoionization). Here an atom absorbs a photon that has sufficient energy to cause ionization resulting in an ion and a free electron. Process d, is free-bound emission (photo-recombination). Here an ion and a free electron combine releasing a photon of energy and the resulting atom drops to a discrete bound state. An electron can absorb a photon and go to a higher kinetic energy level (process e) or emit a photon (process f) and drops to a lower energy level. Many a times, a free excited ion collides with another molecule and loses the excess energy in a non-reactive collision. This reduction in the energy level of the ion occurs without emission of a photon (process g) and is termed as quenching.

2.2 Systems Theory Terminology

2.2.1 Linear and Nonlinear Systems

Within the range of a given variable, if the response of the system satisfies the properties of superposition and homogeneity, the system is considered to be linear, else it is defined as a non-linear system.

2.2.2 System Representation

In terms of control theory, two different means of representation are of interest, namely the input-output relation method and the state-variable method. These two means of representation differ more in degree than in nature. To be more precise, the input-output relation method provides less detail and therefore is less complete than the state-variable method.

2.2.3 Transfer Functions and Block Diagrams

One of the principal tools of the input-output representation is the transfer function. The idea of using the transfer functions to represent physical systems is a natural outgrowth of the use of Laplace transform operational methods to solve linear differential equations. These operational methods have been so successful in simplifying and systematizing the problem of obtaining the time response of a system that it appears reasonable that they should also be valuable in system representation of flame dynamics.

A transfer function is defined as a ratio of the Laplase transform of the output to the Laplase transform of the input, with zero initial conditions. A transfer function may be defined only for a linear, stationary (constant parameter) system. A non stationary system, often called a time-varying system, has one or more time-varying parameters, and the Laplace transformation may not be utilized. Furthermore, a transfer function is an input-output description of the behavior of a system. Thus the transfer function does not include any information concerning the internal structure of a system and its behavior. Thus in the frequency domain, a transfer function relates the output of a system to its input. This can be written as

$$\frac{y(s)}{u(s)} = G_p(s) \tag{2.6}$$

where $y(s)$ is the output from the system while $u(s)$ is the input to the plant, and $G_p(s)$ is the transfer function. This can be expressed pictorially as shown in Figure 2.3, a technique called the block diagram method.

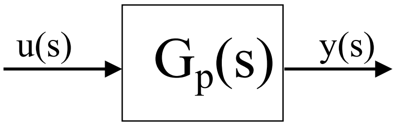

Figure 2.3: Block diagram representation of the input-output relationship

Therefore, the describing set of differential equations, the transfer function and the block diagram are three equivalent forms of representing a system and together constitute what is loosely referred to as the input-output method of plant representation.

2.2.4 Poles and Zeros

The denominator polynomial $u(s)$ in equation 2.6 is called the characteristic equation because its roots determine the character of the time response. The roots of this characteristic equation are known as the poles or singularities of the system. The roots of the numerator polynomial $y(s)$ are called the zeros of the system. The zeros are the conditions in the frequency domain when there will be no response from the system.

2.2.5 Damping Ratio, Resonant Frequency and Natural Frequency

The number of roots of the characteristic equation define the order of the system. Consider a second order system. Its characteristic equation is a quadratic algebraic equation in the 'S' plane that can be written as

$$s^2 + 2\zeta\omega_n s + \omega_n^2 = 0 \tag{2.7}$$

where ω_n is the natural frequency of the system, and ζ is the damping ratio.

The roots of the equation 2.7 are

$$s_1,\ s_2 = -\zeta\omega_n \pm \omega_n\sqrt{\zeta_2 - 1} \tag{2.8}$$

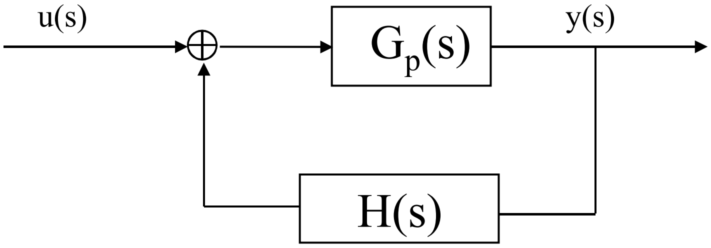

Figure 2.4: Block diagram representation of a closed loop system

For $\zeta \geq 1$, the roots are real; for $\zeta < 1$, the roots are complex and the system exhibits resonance at a frequency of $\omega_n\sqrt{\zeta_2 - 1}$, which is called the resonant frequency of the system. For $\zeta = 0$, the resonant frequency of the system matches the natural frequency of the system. For $\zeta = 1$, there are two real repeated roots. This condition is called the critical damping

2.2.6 Open and Closed Loop Systems

Whenever the output of the system does not effect its input, it is termed as an open loop system, as shown in Figure 2.3. When we have a situation that the output of the system actually effects the input, we have a closed loop system and the situation is termed as feedback of the output signal. This is schematically shown in Figure 2.4. A closed loop system is classified as a negative feedback system if the output is fedback after inverting its sign. If the output effects the input signal without a sign inversion, the condition is termed as a positive feedback system.

2.2.7 Frequency Response Function

Let us consider the time response of a rather general linear system driven by the sinusoidal time function $r(t) = Asin(\omega t)$, as seen in Figure 2.5. The output is $y(t)$, and the transfer function of the system is $W(s)$, where $W(s)$ is assumed to be a ratio of polynomials in s. The output $y(t)$ contains, among other things, a sinusoidal component of the same frequency

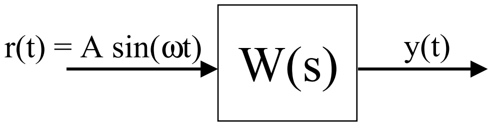

Figure 2.5: General linear system with sinusoidal input

as the input of the form $AR(\omega)sin[\omega t + \phi(\omega)]$. Here $R(\omega)$ is the ratio of the magnitude of the sinusoidal component of the output to the sinusoidal component of the input, and the phase angle $\phi(\omega)$ is the phase difference between the input and the output. Both R and ϕ have been designated as functions of ω since, in general, they vary as the input frequency is varied. It can then be proven that

$$R(\omega) = |W(s)||_{s=j\omega} = |W(j\omega)| \tag{2.9}$$

$$\phi(\omega) = phase\, angle\, of\, W(s)\,|_{s=j\omega} = argW(j\omega) \tag{2.10}$$

This means that the magnitude and the phase of the output for a sinusoidal input may be found by simply determining the magnitude and the phase of $W(j\omega)$. The complex function $W(j\omega)$ is referred to as the frequency-response function. The proof of the above statement can be found in [14].

Based on the characteristics of a frequency response function, it can be stated 'The frequency response function of a linear system uniquely determines the time response of the system to any known input' and 'The frequency response function of a linear system is uniquely determined by its time response to any known input'.