1
Introduction

This chapter presents a brief introduction of the applications of combustion phenomena to industrial processes, followed by the objectives and outline of this dissertation.

1.1
Historical and Economical Aspects

The combustion process is present in the history of mankind since the beginning of the first civilizations. The ability to control fire allowed significant changes in early humans lives. Mankind uses fire as a source of heat and light, which made possible to cook food, to stay warmed during the nights and cold weather, to keep the wild animals away, etc. Today, combustion plays a key role on the evolution and development of the modern civilization. Around 92% of all energy produced in the planet and 81% of the energy produced in Brazil uses combustion phenomena based processes (EPE, 2009) [16].

Table 1.1 shows the energy supply structure in Brazil in 2008 and in the world in 2007. From these data it is possible to see that a predominance exists of the processes that use combustion (biomass, coal, natural gas and oil and oil by-products) for energy production.

Table 1.1: Energy supply structure by source for Brazil in 2008 and World in 2007 (EPE, 2009) [16].

Source	Brazil (%)	World (%)
Biomass	28.6	9.8
Coal	5.8	26.5
Hydraulic and Eletric Energy	14.0	2.2
Natural Gas	10.3	20.9
Oil and Oil by-products	36.6	34.0
Other	3.4	0.7
Uranium	1.5	5.9

1.2 Combustion Applied to Industrial Devices

Combustion has a unique role in industrial and household applications. Some of the industrial and household devices that use combustion process on their operation are industrial process furnaces, burners, boilers, gas turbines, internal combustion engines, natural gas heaters, etc.

1.2.1 Industrial Process Furnaces

Industrial process furnaces are used, for example, as reactor and/or source of heat for the chemical reactions present in the refining and petrochemical industries. The design of these reactors should consider their function, mechanism of warming, fuel type and the oxidizer injection mechanism. Several industrial furnaces have major common characteristics, as represented in Figure 1.1 where a furnace and its process are shown.

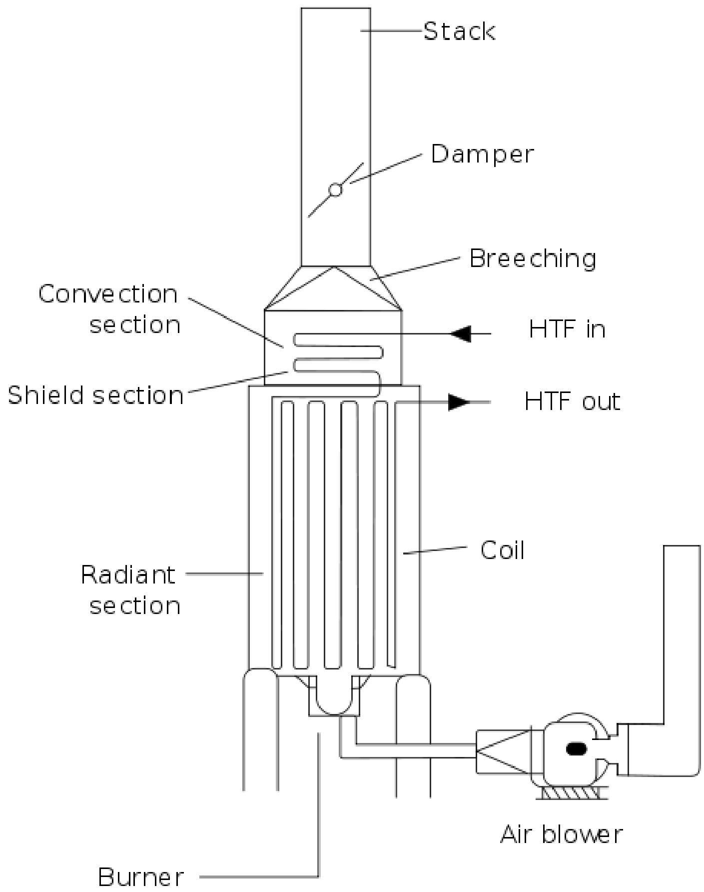

Figure 1.1: Schematic representation of an industrial process furnace. Adapted from `http://en.wikipedia.org/wiki/Furnace`

The fuel enters the burner and it is consumed along with the air supplied by the blower. At certain types of furnaces it is possible to find more than one burner, which can be arranged in cells, for instance. The burners may also be mounted on the floor, on the wall or on the ceiling of the oven (Baukal Jr. & Schwartz, 2001) [3].

In the radiant section, where combustion occurs, the flame heats the pipe, transferring heat to the fluid in its interior mainly by a radiative exchange mechanism (Baukal Jr. & Schwartz, 2001) [3]. The working fluid passing through tubes is heated until the desired temperature is reached. Downstream to the radiant section there usually exists a section where most of the heat is recovered by convection before the gases are expelled.

1.2.2 Gas Turbines

Gas turbines are rotating machines that convert energy from combustion process of an internal gas flow into electrical power, for instance. The gas turbine is designed to operate according to a Brayton cycle in which, firstly, the air is compressed isentropically, then, in a second stage, the pressurized air receives heat via the combustion process that occurs at constant pressure, next, the heated-pressurized air undergoes an isentropic expansion which takes the air to its initial pressure and, finally, the heated air is cooled to its initial temperature through a isobaric process.

The Figure 1.2 presents a sketch of a reverse flow combustor gas turbine. In the combustion chamber, fuel and air are mixed ignited. As a consequence, both the temperature and the specific volume of the gas increase, resulting in a flow velocity increment, which is directed to the expansion turbine blades.

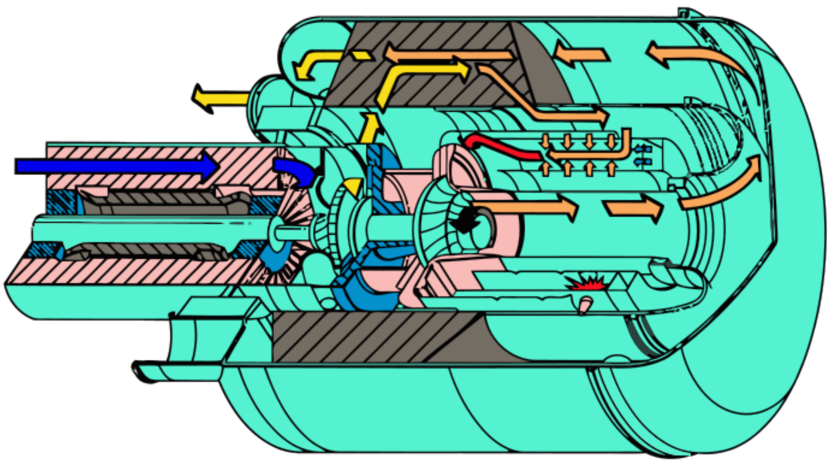

Figure 1.2: Sketch of reverse flow combustor gas turbine. Adapted from `http://en.wikipedia.org/wiki/Capstone_Turbine`

The energy resulting from this process may be extracted as axis work, compressed air or thrust, being used to supply systems such as aircrafts, ships, trains, electric generation plants, etc.

1.3 Fundamental Challenges

Most of the engineering problems related to combustion in industrial applications, regarding design and optimization of devices such as those described above, can be synthesized into two main aspects: energy efficiency and environmental control. Energy efficiency is the aspect related to the improvement of the thermodynamical performance of the process in which apparatus of interest operates, and may be summarized as the production of more outcome spending less energy. Environmental control is the aspect related to the decreasing of pollution generated by the process of fuel burning, in particular to the reduction of the emissions of chemicals harmful to human health or responsible for the greenhouse effect, such as nitrogen oxides (NO_x), carbon dioxide (CO_2) and soot.

Thermodynamical optimization devoted to obtaining a cleaner burning — with a lower level of pollutants emissions — is a multidisciplinary task that requires basic knowledge of thermodynamics, fluid mechanics and heat transfer. Besides the basic understanding of physical processes, to obtain solutions with the required accuracy for certain applications, sophisticated numerical techniques are increasingly used as predictive tools. The development of these techniques and their viable implementation, so that the solutions are obtained with the required precision in an acceptable time, is a challenging research area.

In the modeling of chemically reactive flows, difficulties are encountered due to the characteristics inherent to the complex nature of the combustion phenomenon. Furthermore, nearly all chemically reactive flows with practical applications operate in the turbulent regime. The modelling of combustion/turbulence interactions is an open problem, even after four decades of sustained research (Peters, 2009) [67].

In order to correctly predict the behavior of complex chemically reactive flows, the use of the large eddy simulation (LES) technique, coupled with a reaction mechanism that realistically describes the combustion process, is perhaps the most promising development. In particular, such a development requires two ingredients: a comprehensive detailed reaction mechanism and methodologies to reduce the reaction mechanism cost of use and stiffness (Lu & Law, 2009) [55].

1.4 Objectives of this Dissertation

The computational models for chemically reactive flows are very expensive in terms of time processing. These models demand the evaluation of the rate of reaction of the chemical species, which is a difficult task, in terms computer performance, due to numerical stiffness and its nonlinear nature. This dissertation aims to develop a technique to reduce the time complexity associated to the modelling of turbulent chemically reactive flows with detailed thermochemistry.

Techniques for reduction of reaction mechanisms and for efficient computation of the chemically reactive flows models with detailed thermochemistry are presented in this work throughout a literature review. The method dubbed *in situ* adaptive tabulation is implemented and tested in the simulation of stirred reactor models in order to evaluate its potential as an efficient strategy for the computation of realistic combustion thermochemistry in LES calculations.

1.5 Outline of this Dissertation

This dissertation is composed of seven chapters and three appendices. The second chapter presents a literature review of the existing techniques to reduce the size of a reaction mechanism and efficiently solve a chemically reactive flow model with detailed thermochemistry. The third chapter gives an overview of the fundamental aspects of modelling of stirred reactors. The fourth chapter presents a numerical procedure to integrate the governing equations of stirred reactors models. The fifth chapter develops the theory of the *in situ* adaptive tabulation. The sixth chapter describes the verification tests and the simulation results for a partially stirred reactor subjected to different parameters and reaction mechanisms. The seventh chapter summarizes the contributions of this dissertation, its main conclusions and suggests some paths for future works. The first appendix presents the procedure of construction of the dimensionless parameters. In the second appendix is shown the analysis of efficiency for *in situ* adaptive tabulation algorithm. Finally, the third appendix presents a conference paper which summarizes the main results of this dissertation.