Available online at www.sciencedirect.com

ScienceDirect

Proceedings of the Combustion Institute 36 (2017) 1637–1644

Proceedings of the Combustion Institute

www.elsevier.com/locate/proci

A criterion to distinguish autoignition and propagation applied to a lifted methane–air jet flame

O. Schulz [a,*], T. Jaravel [b], T. Poinsot [b], B. Cuenot [b], N. Noiray [a]

[a] *CAPS Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, Zurich 8092, Switzerland*
[b] *CERFACS, 42 Avenue G. Coriolis, Toulouse Cedex 01 31057, France*

Received 3 December 2015; accepted 7 August 2016
Available online 10 October 2016

Abstract

This numerical study deals with the distinction between autoignition and propagation driven reaction zones using an autoignition index (*AI*). It allows a clear identification of the two burning regimes based on the relative contribution of two reactions for hydroperoxyl (HO_2) chemistry. *AI* was applied to a lifted methane–air jet in a hot (1350 K) vitiated coflow, namely the Cabra flame configuration. Large Eddy Simulation (LES) were performed using the Dynamic Thickened Flame model (DTF) with an Analytically Reduced Chemistry (ARC) mechanism with 22 transported species, as well as 18 species in Quasi-Steady State (QSS) approximation. A detailed validation of the numerical methods is presented. Comparisons with experimental data are in good agreement for mixture fraction, temperature and species mass fractions for both a fine and a coarse mesh. In a detailed analysis of the flame structure, *AI* identifies autoignition as dominant over propagation at the flame base. Autoignition pockets are close to the lean most reactive mixture fraction. Lean and rich propagation is recognized to dominate in regions located at higher mixture fractions closer to the centerline with significantly higher heat release rates compared to autoignition.

Keywords: Autoignition; LES; Lifted flame; Thickened flame model; Reduced chemistry

1. Introduction

The design complexity of modern combustors is constantly increasing – for example in land-based gas turbine applications, sequential combustion or axial staging concepts [1–3] involving Moderate or Intense Low-oxygen Dilution (MILD) [4], or Exhaust Gas Recirculation (EGR) architectures [5]. These technology step-changes are driven by the demand for lower pollutant emissions, higher efficiency and higher fuel and operational flexibility. Recent progress in experimental methods and in Computational Fluid Dynamics enable more robust design and optimization of these new concepts. Still there are often situations, for instance, during prototypes testing phases, where a qualitative and quantitative understanding of the combustion process is lacking. The combustion regime in practical systems is one of these important questions, as premixed

* Corresponding author.
E-mail address: oschulz@ethz.ch (O. Schulz).

http://dx.doi.org/10.1016/j.proci.2016.08.022
1540-7489

Table 1
Numerical studies applied to the Cabra flame classified according to their combustion model (PDF – Probability Density Function, CMC – Conditional Moment Closure, TF – Thickened Flame).

		PDF	CMC	TF
Tabulated Chemistry	RANS	[15–17]	[11]	–
	LES	[12,18–20]	–	–
Full Chemistry	RANS	[22]	–	–
	LES	–	[23]	–
Reduced Chemistry	RANS	[13,24]	–	–
	LES	–	[25]	**This Work**

or partially-premixed propagation, non-premixed combustion or autoignition, have a direct impact on the performances and stability of the burner.

With the aim of distinguishing between premixed and non-premixed flames, Yamashita et al. [6] derived the flame index (*FI*). Another criterion is proposed in this paper, that allows to discriminate between propagating and auto-igniting reaction zones. It is built on the reaction rate flux analysis proposed by Yoo et al. [7], who identified the dominant role of autoignition at the flame base of a hydrogen jet flame by analyzing the chemistry of hydroperoxyl (HO_2) and hydroxyl (OH). This is particularly relevant for flames stabilized in vitiated flows encountered for instance in modern turbomachinery applications – one can refer to previous experimental work [8–10] or numerical studies [7,11,12] on that topic. The here proposed criterion was applied to the lifted methane–air jet, that has been experimentally and numerically investigated by Cabra et al. [13].

This well-documented experimental work has been used for development and validation purposes of several combustion models, summarized in Table 1. The widely used tabulated flamelet approach originally proposed by Peters [14] has been providing encouraging results for Reynolds-averaged Navier–Stokes (RANS) [15–17] and Large Eddy Simulation (LES) modeling [12,18–20]. However one drawback is the augmented complexity of the look-up table with more practical combustion applications. Cooling, dilution or fuel injection with different compositions can result in three or higher stream mixing problems, adding a number of parameters to the look-up table and therefore considerably increasing the computing time [21].

As an alternative, a 44 species detailed chemistry scheme, combined with a transported Probability Density Function (PDF) was used by Gkagkas and Lindstedt [22] in RANS simulations. Their work gives insight into the dominant reactions for the pre- and autoignition process. Martinez and Kronenburg used a detailed skeletal mechanism with 44 species [23] and reduced mechanisms [25], both in combination with a CMC approach to perform LES. Such methods still lead to important computing time to resolve the stochastic nature of the reacting turbulent flow.

In the present paper, for the first time the Thickened Flame (TF) model [26] in combination with reduced chemistry is used to simulate the Cabra flame. Objectives are to evaluate the performances of this less demanding approach in terms of computing time, and to analyze the flame structure in view of identifying the combustion regimes.

The current paper is structured as follows: In the following section, the criterion to distinguish between autoignition and propagation is presented. In the third section, the Cabra flame configuration is introduced and numerical approaches are validated against the experiment. In the last part, the autoignition index (*AI*) is applied to the Cabra flame configuration and an analysis of the flame structure and stabilization mechanism is proposed.

2. A criterion to distinguish between autoignition and propagation

A reaction rate flux analysis of HO_2 chemistry to distinguish between propagation and autoignition is presented. This analysis is based on the findings of Gkagkas and Lindstedt [22], who showed that the formation of the HO_2 radical is mainly due to (keeping the same reaction numbering as in [22]):

$$O_2 + H(+M) \Longleftrightarrow HO_2(+M) \quad \text{(R5)}$$

$$CHO + O_2 \Longleftrightarrow CO + HO_2 \quad \text{(R34)}$$

Consumption of HO_2 is through the following reactions:

$$HO_2 + H \Longleftrightarrow OH + OH \quad \text{(R6)}$$

$$HO_2 + OH \Longleftrightarrow H_2O + O_2 \quad \text{(R8)}$$

$$CH_3 + HO_2 \Longleftrightarrow CH_3O + OH \quad \text{(R74)}$$

Figure 1 shows the HO_2 reaction rates ($\dot{\omega}_{HO_2}$) profiles of the above reactions for three different 1-D simulations representing different burning regimes, namely propagation (a) and autoignition (d), as well as a transitional case between the two (c). Indeed, below a minimum equivalence ratio a freely propagating flame cannot be observed anymore and autoignition of the fresh mixture starts to dominate [12]. Note the change in spatial scale between propagation and autoignition regimes. The 1-D propagating laminar flame (a) is stabilized by imposing the velocity of the laminar flame speed $s_L = 3.2$ m/s at the inlet, whereas the position of the reaction zone of simulation (d) is determined by the inlet velocity and the autoignition time of the mixture imposed at the inlet. The inlet velocity