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Chemical structure of autoignition in a turbulent lifted H_2/N_2 jet flame issuing into a vitiated coflow

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ABSTRACT

In the present paper autoignition is studied as the main stabilization mechanism in turbulent lifted H_2/N_2 jet flames issuing into a vitiated hot coflow. The numerical study is performed using the joint scalar PDF approach with detailed chemistry in a two dimensional axisymmetric domain. The SSG Reynolds stress model is used as a turbulence model in the simulation. Chemical structure and characteristics of autoignition are investigated using various methods and parameters. Reaction rate analysis is made to analyze the ignition process at the flame base. The results show the occurrence of a chain branching reaction preceding thermal runaway, which boosts the chain branching process in the flame. This demonstrates the large impact of autoignition at the flame base on the stabilization of the lifted turbulent flame. Further investigation using the scatter-plots of scalars reveals the characteristics of the ignition. The relation between the behavior of temperature and of key intermediate species demonstrates the formation of OH through consumption of HO_2 at nearly isothermal conditions in a very lean-fuel mixture at the flame base. Flux analyses in the conservation equations of species are used to explore the impacts of mass transport on ignition process. Ignition is found to be mainly controlled by chemical features rather than the mixing processes near the flame base. Characteristics of autoignition are also investigated in terms of Damköhler number and progress variable.

1. Introduction

Increasing demand for high power/low emission devices and the trend toward using of low grade fuels have made flame stabilization a more important issue in recent years. Pilot, swirl and bluff-body stabilized flames are widely used to achieve flame stabilization in practical combustors and furnaces. In these flames, the combustion products are usually mixed with the cold reactants creating a continuous ignition. To investigate the mechanisms controlling the flames in an environment of hot gases, *Jet-in-Hot-Coflow* (JHC) flames have been used as they can properly emulate the conditions in non-premixed or partially-premixed jets in hot coflow of the post combustion gases. JHC flames show many features of turbulence-chemistry interaction in the recirculation regions of advanced combustors while the flow pattern is simplified by eliminating the complex recirculating fluid mechanics. The turbulence characteristics in recirculating flows in general cannot be modeled as accurately as in the jets and shear flows. The deficiencies of the turbulence models can be less than required to address questions on turbulence-chemistry interaction and make the evaluation of sub-models more difficult. This problem is resolved to a great extent by employing the JHC flames and fundamental investigations become possible to gain more understanding of flame stabilization. Simplicity in the flow pattern of the JHC flame nevertheless allows exploration of the flame for different fuels and under a variety of different operating conditions which can be the representative of different regions inside combustion devices. Based on the previous studies [1–7], parameters which are recognized to be the most influential on JHC flames are coflow temperature, velocity for both jet and coflow streams and oxygen content of coflow. These parameters can be used to categorize the JHC flames and to examine the viability of different modeling approaches.

Turbulent lifted jet flames in a cold environment have been widely investigated due to importance in practical applications. Despite the simplicity of the flow, various theories have been proposed to explain the stabilization mechanism of the turbulent lifted flames [8,9]. In general, theories can be classified into two

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main groups based on the degree of premixing upstream of the flame base and the local turbulence structure near the flame base. Theories based on the first group are premixed flame theory [10,11], non-premixed flamelet theory [12] and edge flame theory [13–17] while the second group includes turbulence intensity theory [11,18] and large eddy theory [19,20].

For turbulent lifted jet flames in a hot coflow, autoignition has been proposed as another stabilization mechanism. The presence of autoignition in JHC flames has been confirmed by numerous experimental and numerical studies [7,21–23]. By analyzing the flame luminescence with an intensified high-speed camera, Oldenhof et al. [5,24] investigated the lift-off behavior of flames burning in both hot and cold coflows. Analysis of the luminescence images showed that the physical mechanisms governing the lift-off process in jet-in-hot-coflow flames and conventional lifted flames are fundamentally different. The difference is reflected in the sensitivity of lift-off height to the Reynolds number. The occurrence of autoignition at the flame base of jet-in hot-coflow was studied numerically by Gordon et al. [2,25]. They employed the joint scalar probability density function (PDF) approach with detailed chemistry and in this framework they analyzed the species transport with respect to the budgets of convection, diffusion and reaction near the flame base. They showed that when reaction is balanced by convective term with minimal contribution of axial diffusion, auto-ignition can provide flame stabilization. On the other hand, a diffusive-reactive balance, preceded by a convective-diffusive balance indicates stabilization by premixed flame propagation. They also showed that the creation of certain radical species such as HO_2 ahead of the flame zone can be used as another indicator of autoignition. Flame structure in lifted flames in a hot coflow was further analyzed using Reynolds-Averaged Navier–Stokes-Conditional Moment Closure (RANS-CMC) approach with detailed chemistry by Patwardhan et al. [26]. Profiles of mean scalar fluxes in mixture fraction space reveal that the chemical reaction term balances the molecular diffusion term inside the flame zone while in the pre-flame zone, the structure depends on the coflow temperature. They concluded that the lift-off height is controlled by autoignition and turbulent premixed flame propagation depending on the coflow temperatures. Yoo et al. [27] employed a 3-D direct numerical simulation with detailed chemistry to show which mechanisms are controlling the flame stabilization in turbulent lifted jet flames. They performed a detailed analysis using Damköhler number, the relative locations of key intermediate-species and chemical reaction rate analysis. Autoignition was found as the main source of stabilization occurring in the fuel-lean mixture at the flame base. They also concluded that downstream of flame base, both rich premixed and non-premixed flames develop and coexist with autoignition. Lagrangian tracking of the flame base showed the existence of large-scale structures leading to fluctuations at the flame base. More recently, a combined Large Eddy Simulation-Conditional Moment Closure (LES-CMC) approach was used to analyze the flame stabilization in a wide range of lifted flame geometries by Navarro-Martinez et al. [28]. It was found that LES-CMC with conditioning on mixture fraction can predict the different stabilization mechanisms using the analysis of the transport budgets. Depending on the coflow temperature, autoignition and premixed flame propagation were introduced as the mechanisms of flame stabilization in the lifted jet flames. Using LES-CMC in a hydrogen lifted flame in the hot coflow, Stanković et al. [29] also showed the role of turbulence and mixing in the location of autoignition. They found that stronger turbulence could promote the ignition.

Understanding autoignition is of fundamental importance for practical applications, particularly for combustion engines and gas turbines. The role of turbulence, finite chemistry and scalar dissipation has been the subject of several studies and detailed information regarding the contributions of these parameters has been obtained using direct numerical simulations (DNS) [30–34]. The two dimensional DNS study with a single step hydrogen chemistry by Mastorakos et al. [30] showed that autoignition in a shear free mixing layer between hot oxidizer and cold fuel does not necessarily occur at the stoichiometric mixture fraction but rather at a mixture fraction where the fluid is most reactive. This most reactive mixture fraction is determined by the competition between the effect of high temperature (in the coflow) and reactant concentrations (stoichiometric conditions). They also showed that autoignition most likely occurs at low scalar dissipation rates and thereby the regions with low heat losses. In terms of the effect of turbulence, they also showed that the ignition delay is not sensitive to the turbulence time scale, t_{turb} in the range of $t_{ign} < t_{turb}$ which is consistent with the results obtained in [34]. On the other hand, the two dimensional direct numerical simulation with detailed chemistry for hydrogen-oxidation by Im et al. [31] showed a non-monotonic behavior for ignition delay versus turbulence intensity. For moderate turbulence, ignition is facilitated via enhancing the mixing, while for stronger turbulence, ignition is retarded due to excessive scalar dissipation.

Autoignition is a transient process initiated from a slowly reacting state and eventually leading to a fully burning state corresponding to the combustion at high temperature. The reactions that control autoignition can be different from those in high temperature combustion [35] and correct representation of the finite rate effects during autoignition is critical. Investigation of the case of hydrogen flames is useful for understanding the autoignition process since the chemistry is more accurately known than the chemistry of hydrocarbon fuels and at the same time forms a part of the chemistry of those fuels. Ignition in hydrogen–oxygen combustion consists of two stages. The first stage of ignition is the induction stage which occurs under nearly isothermal condition during which radicals build up. The second stage is characterized by transition to high temperature combustion and is referred as thermal runaway. The role of finite rate chemistry of hydrogen oxidation in ignition for non-premixed counter-flowing jets of fuel against heated air has been investigated by Kreutz and Law [36]. They showed that the ignition of diffusive systems follows the same behavior as those observed in explosion limits of homogeneous mixtures. Further studies regarding the coupling effect of chemistry and scalar dissipation rate have been performed by Echekki and Chen [37]. By two dimensional direct numerical simulation with detailed chemistry, they showed that the evolution of ignition kernels is characterized by the strong coupling at the ignition kernels of dominant chemistry, responsible for the growth of radical pool, and thermal and intermediate species losses due to dissipation.

To study the influence of chemistry on auto-ignition and subsequent development of turbulent lifted flames in the framework of turbulent combustion models, both the accuracy of the chemical mechanism and the use of an appropriate turbulence-chemistry interaction models are essential. A variety of modeling methods have already been evaluated for representing the highly non-linear interaction between turbulence and chemical reaction in lifted flames in hot coflow using RANS type simulations [38,26,39–43] and LES type simulations [44–46,28,47–50]. Among them, transported PDF methods have the advantage of representing reaction exactly without modeling assumptions. These methods have been applied in computational studies of experiments by Cabra et al. in Refs. [21,3,51,1,52,25,53–55]. The simulation using the RANS-joint scalar PDF method with detailed chemistry by Masri et al. [51] has shown that the results are very sensitive to the chemical mechanism used and that the flame is largely controlled by chemical kinetics rather than mixing process. An important feature of this flame is the strong sensitivity of lift-off height to the coflow tem-