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A new reduced kinetic mechanism for turbulent jet diffusion flames of bioethanol

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ABSTRACT

In the last years, the understanding of the biofuels combustion processes has been facilitated through the progress of asymptotic methods, due to the difficulty of simulating the large number of reactions and species involved in the combustion. To model the molecular mixing and the combustion of a turbulent jet diffusion flame of bioethanol was using a model based on the equations of Navier–Stokes, mixture fraction, mole fraction of species and enthalpy, which are written following the large-eddy simulation approach. The Eulerian formulation is used to solve the equations governing the gas phase. The effect of the droplets of the liquid phase is considered by the introduction of appropriate source terms in the equations of the gas phase. To decrease the stiffness of the reactive system of equations, a reduced kinetic mechanism of bioethanol is developed. The reduced mechanism obtained is tested to simulate a turbulent jet diffusion flame and the results compare favorably with data found in the literature. The reduced mechanism can facilitate the work of researchers in this field, because the methodology developed allows decreasing considerably the time needed to obtain reasonable results for confined turbulent jet diffusion flames of bioethanol.

1. Introduction

The term biofuel is referred to as solid, liquid, or gaseous fuels that are predominantly produced from biorenewable or combustible renewable feedstocks [1]. Liquid biofuels are important for the future because they may replace petroleum fuels. Biofuels are generally considered offer many priorities, including sustainability, reduction of greenhouse gas emissions, regional development, social structure and the agriculture, among others [2]. The biggest difference between biofuels and petroleum feedstocks is oxygen content.

Ethanol is the most widely used liquid biofuel. It is an alcohol and is usually fermented from sugars, starches, or cellulosic biomass. It is used as a renewable energy fuel source as well for the manufacture of cosmetics, pharmaceuticals, and also for the production of alcoholic beverages. Therefore, we need a good understanding of the reaction pathways by which bioethanol is oxidized and of the pollutant species that it may produce. This understanding enables industry and regulatory agencies assess the viability and the relationship between the combustion process and pollutant emissions when using the bioethanol.

The chemical kinetic modeling has become an important tool for interpreting and understanding the phenomena of combustion. Its application requires as an input a valid chemical reaction mechanism [3]. However, models of combustion may become very complex. For the oxidation of hydrogen, for example, are often used 9 species and 19 elementary reactions [4].

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The mechanism of combustion of methane, the most simple of the hydrocarbons, presents more than 300 elementary reactions and 30 species [5]. Marinov presented a detailed mechanism for the ethanol combustion at high temperature containing 372 elementary reactions [6]. Saxena and Williams investigated the combustion of ethanol based on a chemical kinetic mechanism consisting of 192 elementary reactions and 36 species, with the addition of 53 reactions and 14 species to address the formation of nitrogen oxides and 43 reactions and 7 species to address the formation of compounds involving three carbon atoms [7]. The oxidation of iso-octane includes 3600 elementary reactions among 860 chemical species [8].

Numerical computations to solve the chemical kinetics equations of combustion systems for species concentration evolution often require significant computational time. This occurs for even the simplest models. When the kinetics equations are solved in addition to conservation equations for complex flow models, the computational time may become excessive and not practical. Therefore, techniques for reducing the kinetic mechanisms can be applied and to facilitate its resolution.

There are several strategies for reducing calculations necessary to obtain the kinetics description of a combustion system. In the last decades, the reduced chemistry has been employed to describe flame structures. The systematic reduction of the chemistry is achieved by introducing appropriate steady-state or partial-equilibrium approximations into detailed chemistry and neglecting terms and reactions of lesser importance to achieve simplified descriptions of the flame structure [9]. This technique is not new, it has been known since the works of Peters [10], Seshadri et al. [11], and many others.

In addition to the steady state and the partial equilibrium assumptions, other methods have emerged with the same purpose, as the Intrinsic Low-Dimensional Manifolds (ILDM) method, where the slow and fast processes are separated based on analysis of the Jacobian matrix of the chemical source term [12]. The Reaction Diffusion Manifolds (REDIM) method corresponds to an evolution of the ILDM method [13,14] and it is based on the solution of an equation to obtain a low-dimensional manifold in the kinetic space. This method eliminates many of the deficiencies of the ILDM concept, because it takes into account the coupling of reaction and molecular transport processes.

Currently, the study, the analysis and the understanding of the phenomenology of the most burning flows are developed through computer modeling and laboratory experiments. Through numerical simulation we can create computational models for situations where it is impossible or very expensive to test or to measure the various possible solutions of a phenomenon from experimental models and analytical solutions. It is known that, in some cases, the numerical solution induces flow characteristics not before realized in experiments.

The coupling between chemistry and turbulence creates a large field of research. One of the most common techniques used to analyze turbulent flows is the large-eddy simulation (LES), as can be seen in the work of Boersma and Lele [15], Rawat et al. [16] and Sheikhi et al. [17], among many others. The large-eddy simulation technique resolves or directly obtains all large scale structures of the flow and requires models for the small-scale or unresolved features of the flow. Typical combustion chemistry occurs at length scales far smaller than the resolved length scales in practical simulations. Thus, the combustion process occurs essentially at the smallest scales, and has to be modeled entirely [18].

The turbulence can affect the flow in profound ways, so it is common to find significant differences between the Direct Numerical Simulation (DNS) and the LES predictions. This leads to the possibility to use LES in coarse meshes as a tool for determining the gross features of the flow [19].

In this work we use the finite difference method with the large-eddy simulation to model a flame of bioethanol. The advantage of using these methods is that they are comparatively economical in the assembly of the system of equations due to the simplicity of the operations involved, which is why such schemes are widely used. Using the steady state and the partial equilibrium approximations, a reduced kinetic mechanism was developed to decrease the rigidity of the system of equations.

2. Obtainment of reduced kinetic mechanism

The combustion of bioethanol is investigated here using a skeletal chemical kinetic mechanism consisting of 372 elementary steps among 56 species [6]. Theoretically, for each species necessary to solve a differential equation. Thus, reduced kinetic mechanisms are conveniently used. The reactions of a mechanism contains various characteristic properties and the knowledge of these properties improves the understanding of reactive systems and provides information to simplify the mechanism, by elimination of steps that are irrelevant to the problem of interest. In this work, we reduce the number of reactions and species involved in the system through the elimination of unimportant reactions, based on the assumptions of partial equilibrium and of steady-state.

The justification for the use of the steady-state approximation is generally given in physical terms, because the rate at which the species k is consumed is much faster than the rate by which it is produced, being the derivative of the concentration in time of these species set equal to zero.

$$\frac{d[C_k]}{dt} = 0. \tag{1}$$

The identification of intermediate species at steady-state is realized by the comparison of the magnitude of the specific rate of production and consumption of each species, given by

$$k_{f,r} = B_r T^{n_r} exp\left(-\frac{\Delta E_r}{RT}\right). \tag{2}$$