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REDUCED MECHANISM FOR COMBUSTION OF HYDROGEN AND METHANE WITH NITROGEN CHEMISTRY

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A reduced chemical kinetic reaction mechanism that could be used in computational fluid dynamics (CFD) software was developed to describe the formation of nitrogen oxides and their subsequent destruction in hydrogen and/or hydrocarbon flames with or without seeding of nitrogen compounds. The research work presented here will describe the numerical work done with the application "CHEMKIN" in order to verify the quality of the reduced mechanism. The mechanism was validated through comparisons between computational data from a variety of different sources. In addition, numerical experiments were carried out to examine features of methane combustion in which the detailed mechanisms can be used to compare their response. The proposed reduced mechanism provides reasonable agreement with the studied detailed mechanisms, mainly in the species produced from the hydrocarbon oxidation process. Regarding the produced nitrogen species, the proposed reduced mechanism showed the same tendencies as the detailed mechanisms, but there is a need for a better agreement regarding the quantities.

KEY WORDS: *combustion, reduced mechanism, hydrocarbons, NO_x, CHEMKIN*

1. INTRODUCTION

Certain computational fluid dynamics (CFD) applications, such as the FLUENT software package adopted by the authors in a full 3D reactive flow, have limitations related to the chemical species and reactions to be used. As an example, the above-mentioned application package is unable to support more than 100 chemical species and 500 chemical reactions. There are several detailed kinetic mechanisms that use more chemical species or reactions, and due to these limitations some of them are unable to be used in this CFD application. Moreover, each and every reaction is solved as an independent equation for every control volume on top of the mandatory equations (continuity, momentum, and scalars such as energy), and some additional equations for turbulence and radiation models that will depend entirely on the chosen models. Considering that a computational volume may have several hundred thousand cells to several million cells, all these calculations must be performed for each iteration and most of the cases with reactive flow need thousands of iterations in order to achieve a convergent result. So, besides the limitations in reaction and species number that may be posed by the characteristics of the detailed models, the computational effort will be enormous and may be equivalent to several additional days or weeks.

Therefore some of the available detailed chemical kinetic mechanisms were studied. These mechanisms are summarized below and defined in Table 1. Other detailed mechanisms exist; however, those mechanisms do not address the methane oxidation with nitrogen chemistry. As indicated in Table 1, the main differences among mechanisms are the reactions and the Arrhenius parameters considered. Although all mechanisms address the combustion process, not all of them gave a good response in certain conditions, e.g., the working temperature (2000 K in premixed gas combustion in opposition to 1150 K in a biomass fired fluidized bed combustor).

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