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Effects of Adding Gaseous Soot and Methane Incomplete Combustion Products on Detailed Chemical Kinetics Combustion of Methane and Pollutants

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ABSTRACT: The previous researches show the great effect of soot on natural gas flame radiation. The addition of soot into methane flame is widely proposed by the researchers as a good method to enhance radiation from non-luminous flames. But the effect of adding soot on the chain reactions of methane combustion and NO & CO emission have been not reviewed. The present study investigates the effects of adding gaseous soot on the progress of natural gas combustion and NO & CO emission in the zero-dimensional zone by means of GRI 3.0 mechanism in the Cantera python package. Also, methane incomplete combustion products are considered as an additive to control the pollutants. The results indicate that the addition of gaseous soot into natural-gas flame leads to increase in adiabatic temperature, the rate of decomposition reactions of fuel and brings more CO and NO production. In the other hand, the addition of methane-air incomplete combustion products into natural gas reaction cause to reduce CO production and decrease in the adiabatic flame temperature. So, in order to enhance radiation of methane flame and pollutants reduction the additive that composed of of gaseous soot and methane-air incomplete combustion can be used.

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1- Introduction

The consumption of natural gas can emit 50% less pollution compared to other fossil fuels. The positive role of natural gas in the global energy is increasing, but radiation heat transfer from its blue flame is significantly less than other fuels. Thermal radiation is generally the dominant mechanism, and in particular, soot can play an important role in the radiation heat transfer even in relatively low concentrations. Review of the researches show a number of combustion simulations considering methane/soot chemistry. Rockwell and Rangwala [1] experimentally demonstrated that for a methane-air flame, the addition of coal dust particles to fuel suppresses radiation from the non-luminous natural gas flame. Specific details of the dust injector in such a burner are discussed by Xie et al. [2]. They investigated the interaction of micron-sized coal particles entrained into lean methane–air premixed flames. The results show that the flame temperature reduces with the addition of coal dust having particle sizes in the ranges of 75–90 μm. However, flame temperature promotion is observed for one case with a particle size in the range of 0–25 μm at an equivalence ratio of below 1. Ralf [3] numerically have shown that as the particle size increases their ignition energy increase and the rate of density change is decrease.

Detailed chemical kinetic mechanisms are routinely used to describe at the molecular level the transformation of reactants into products and a complex environment can be broken down via three-dimensional Computational Fluid Dynamics (CFD) calculations, into simplified flow models and detailed chemical kinetics employed. Thus, the current study investigates the combustion of methane with soot particle by employ the GRI3.0 chemical kinetic mechanisms in the Cantera codes. The density change of methane, air, and soot particle are simulated with the ideal gas law. To the best of our knowledge, there is little work on distinguishing the detailed effects of additive C on the formations and consumptions of important species including some soot precursors and oxygenated air pollutants in the CH4-C blended fuels flames. Therefore, in the present study, detailed chemical effects of Carbon addition on methane flames are comprehensively discussed via kinetic analysis. As a reformer, for the emission of pollutions process, the adding of methane incomplete combustion products has studied too.

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2- Methodology

In this study combustion of natural gas as main fuel with air and soot and product of methane incomplete combustion as additive kinetically are investigated. CH_4 and Air (O_2+3.7143N_2+0.04762Ar) was assumed as an ideal gas but there are two ways to model the density change of soot particles in the combustion chamber. As Ralf and Xie et al [2] shown in their literature, we can model the soot density change with a particle size between 0–25 μm by the ideal gas law and for soot with a particle size between 75-90 μm, we can assume constant density. In this paper for modeling the combustion of methane with soot particle, as fuel and air, we use the ideal gas law for soot particle (the case with a particle size in the range of 0–25 μm).

Combustion mechanism was modeled with plug flow reactor (PFR) reactor in the zero-dimensional zone. As Younessi et. al shown for methane combustion with zone temperature above 1500 C the reactions are in an equilibrium state. So the equilibrium equation was used to calculate the adiabatic temperature and mole fraction of combustion species. The detailed chemical reaction mechanism for CH4 oxidation and combustion used here is GRI-Mech 3.0. The mechanism consists of 53 species and 325 reactions. The simple GRI3.0

reaction pathway diagram for combustion of methane in a well-stirred reactor was shown in Fig. 1. The stoichiometric methane–soot–air freely propagated laminar premixed flames at normal temperature and pressure were calculated by using CANTERA code in Python environment. The Cantera package [4] was used to estimate the mole fraction of each species, by solving an adiabatic unstrained premixed laminar flame.

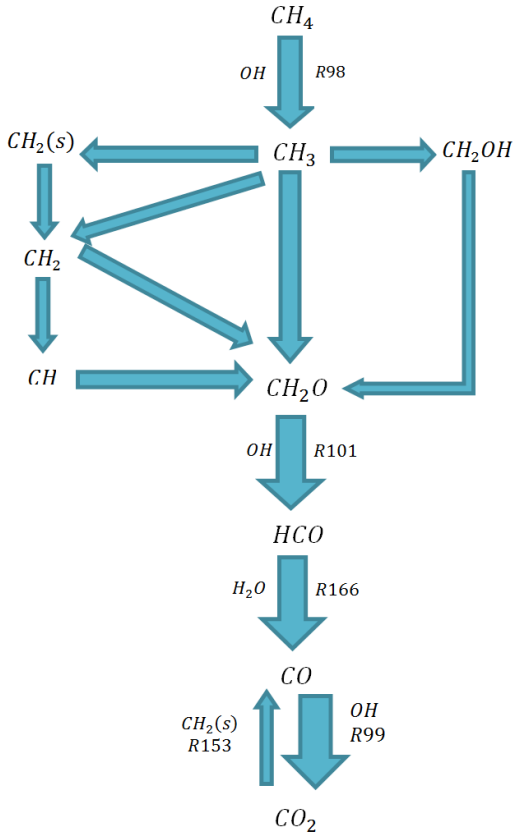

Fig. 1. Reaction pathway diagram for combustion of methane in a well-stirred reactor

3- Results and Discussion

The change of adiabatic temperature and mole fraction all the flame species in the chemical reaction mechanism can be derived from the calculation results. Some representative species including the major species CH_4, CO, CO_2 and intermediate species CH_3, CH_2O, HCO are selected to analyze the effect of soot and product of methane incomplete combustion addition on the methane–air chemical reaction. Meanwhile, the effect of additive addition on NO formation, equilibrium constant and reaction rate of main reactions will also be discussed.

As mentioned earlier, a mathematical model is developed to explain the observation made in the methane/air/soot experiments. The accuracy of the mathematical model is confirmed by comparing the results with the experimental results [5] and numerical simulation [2] which are illustrated in Figs. 2 and 3. GRI-Mech is an optimized detailed chemical reaction mechanism for the calculation of natural gas chemical reaction process. The comparison of the measured adiabatic flame temperature of methane–air mixtures by Lück and G. Tsatsaronis [5] as a function of ϕ with the calculated results with GRI 3.0 in the current model is shown in Fig. 2. Fig. 3 illustrates the comparison of the Xie et al [2] and current model results of the interaction of the soot particles with the premixed methane/air flame on adiabatic flame temperature calculated. Figs. 2 and 3 show a good match of adiabatic temperature between the current model and numerical and experimental results.

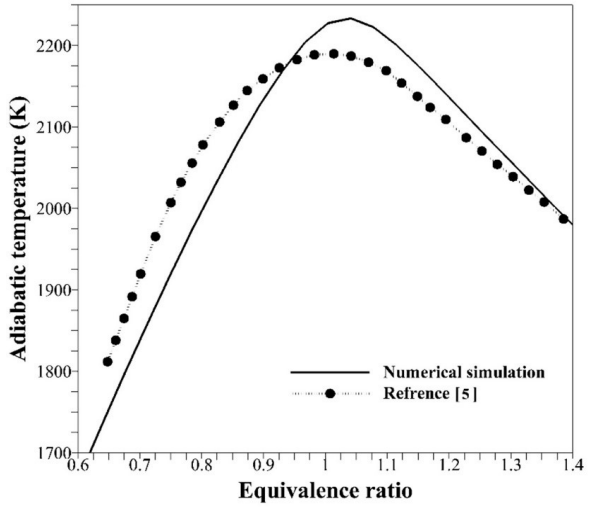

Fig. 2. Reaction pathway diagram for combustion of methane in a well-stirred reactor

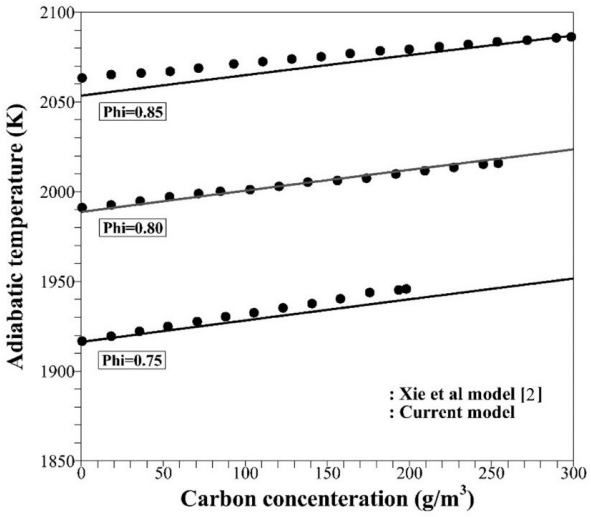

Fig. 3. Reaction pathway diagram for combustion of methane in a well-stirred reactor

4- Conclusions

The kinetic studies of adding soot and methane incomplete combustion products on methane combustion were studied by EPM method with Cantera code in Python environment. The results indicate that:

- the injection of soot into natural-gas flame leads to increase in adiabatic temperature, chain reactions rates and NO and CO pollutions.
- the addition of the product of incomplete combustion of methane into natural gas reaction leads to reduce CO production and cause to lower flame adiabatic temperature.

According to the results, in order to enhance radiation from methane flame and reduction of pollutant's emission the combination of gaseous soot and product of methane incomplete combustion can be injected.

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