A NUMERICAL PREDICTION OF A DILUTED HYDROGEN TURBULENT JET DIFFUSION FLAME USING A SCALAR PROBABILITY DENSITY FUNCTION METHOD CONSIDERING DETAILED CHEMICAL KINETICS

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Keywords: Turbulent Diffusion Flame, Modeling, Probability Density Function Method, Detailed Chemical Kinetics

ABSTRACT

A scalar probability density function (PDF) method considering a detailed chemical kinetics is applied to a diluted hydrogen turbulent jet diffusion flame to evaluate the performance. The flame is formed on a nozzle of an inner diameter of D=6mm, with a fuel exit velocity of 30m/s, surrounded by two annular pipes issuing airs of higher and lower velocities of 30m/s and 3m/s, respectively. The hydrogen as a fuel is diluted by one third volumetrically by the nitrogen, giving a stoichiometric mixture fraction of 0.46. The flow field has been solved on the basis of the k- ε two equation model. A modeled scalar PDF equation has been solved by an Eulerian Monte Carlo method developed by Pope [1]. The PDF transport term due to turbulent velocity fluctuations involved in the PDF equation is modeled based on the gradient diffusion concept. The molecular mixing term is modeled by the modified Curl model [2,3]. On the other hand, reactions are

exactly dealt in the PDF method, because each PDF is able to have the exact information about reactions. A twenty-step reaction, eight species kinetic mechanism for hydrogen-oxygen combustion is employed here. Each scalar joint PDF is described as an ensemble of stochastic particles of thousand at each node. Each PDF is transported through each stochastic process of the turbulent diffusion, the molecular mixing, and the convection.

In order to evaluate the performance of the present PDF method (henceforth, F-PDF), calculation results are compared with those of two flamelet calculations, which are based on the conventional laminar flamelet model (F.M.) method and a scalar PDF (I-PDF) method based on the conserved scalar approach. Calculated velocity fields did not show any important differences that affect the evaluation of scalar fields among these methods. This close estimation for the flow field permits us to discuss only about the scalar field. The F-PDF method has predicted the maximum temperature on the center axis closer to the experimental one than the other methods. The temperature in the downstream of the maximum temperature position however has been overestimated due to the underestimation of mixing. The estimation ability of the F-PDF method has been highlighted in scatter plots of scalar quantities; namely, temperature and species mass fractions, as shown in Fig.1. Solid lines in Fig.1 correspond to the flame structure under the assumption of the infinite reaction rate and one-step irreversible reaction. At x/D=4, scatter plots gather close to the solid lines with slight departures on the rich side. This may reflect the burning under the flame stretch supported by a pilot flame installed around the fuel nozzle, because the departures from the solid lines on the rich side are caused by the flame stretch [4]. At x/D=20, scatter plots collapse into around two regions of the above mentioned flame structure and of the frozen structure

indicated by the straight lines connecting the properties of the fuel and the air before the mixing. Scatter plots around the frozen structure indicate local extinction due to the flame stretch at the location where the support of the pilot flame is weakened. This phenomenon is recognized as bimodal PDF's conditioned on the mixture fraction [5]. At x/D=40, scatter plots again gather to around the fully burning limits, reflecting reignition after the local extinction at the upstream. Moreover, the deviations from the solid lines on the rich side gradually decrease with increasing of x. This shows the strong damping of the flame stretch with increasing x. These results agree qualitatively with experimental results. Consequently, the present PDF method can reproduce the extinction and re-ignition phenomena, which cannot be easily predicted by the conserved scalar approaches (F.M. and I-PDF methods). The variations in the diffusion flame structure due to the flame stretch, which were experimentally confirmed by Barlow et al.[4], have been also reproduced.

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Fig.1 Scatter plots of temperature and mass fractions of species. Solid lines correspond to the flame structure of one-step irreversible reaction.