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NO prediction modeling for numerical simulation of NH3 flame employing flamelet approach

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These days, ammonia has attracted more attention as a carbon-free fuel. Although ammonia combustion does not emit carbon dioxide, it emits more nitrogen oxides (NOx), especially for fuel NOx, compared to conventional fuels [1]. Therefore, the reduction of NOx emissions is one of the most important issues in the development of ammonia-fueled combustors. Since performing numerical simulations of actual-scale combustors with a detailed chemistry is computationally expensive, the application of a combustion model is inevitable. The flamelet approach [2,3] is one of the combustion models widely used.

In the flamelet approach, thermochemical properties are obtained from a pre-tabulated database via control variables. Although the flamelet approach accurately predicts temperature field in the combustor, it has less accuracy for predicting the formation of NOx, which has long chemical time scales. Because of long chemical time scales, it is difficult to summarize NOx-related properties in the database using the reaction progress variable as one of the control variables. To improve the accuracy of NOx prediction, the transport equations of NOx are solved with the NOx formation model (e.g. [4]) in addition to the transport equations of control variables. Although such NOx formation models improve the NOx prediction accuracy, the discrepancies still exist between modeled NOx production rates and actual ones.

Therefore, in this study, a new control variable is introduced instead of directly useing the conventional progress variable as a reference parameter when getting the NOx-related thermochemical properties. The NOx production rates are obtained from the database using a newly introduced control variable, and transport equations of NOx are solved with the referred production rates. The accuracy of the proposed technique is investigated by performing the two-dimensional numerical simulations of an ammonia-air premixed flame at a pressure of 1 atm and unburnt gas temperature of 300 K. Three types of numerical simulations are performed: (1) directly solving the Arrhenius equations in a detailed reaction mechanism, (2) employing the flamelet approach with existing NOx formation model [4], and (3) employing the flamelet approach with proposed technique. The comparisons of numerical results of these three simulations are shown for validation.

References (if needed)

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