Turbulent Diffusion Combustion Model Using Chemical Equilibrium Method Combined with the Eddy Dissipation Concept Model for Simple Prediction of Combustion Products

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This dissertation presents a combustion model that is based on the chemical equilibrium combined with an eddy dissipation concept model (CE-EDC model) for simplifying detailed chemical mechanisms. In the CE-EDC model, the amount of designated chemical species is estimated by calculating their reaction rates using the ED or EDC model. Then, the chemical equilibrium method is used for calculating the amount of the other chemical species on the basis of the assumption that these species are in chemical equilibrium. An advantage of the CE-EDC model is that the amounts of any chemical species can be determined without using detailed chemical mechanisms; it only requires thermodynamic functions. In this dissertation, the CE-EDC model is validated by simulating the H2-air turbulent diffusion flame used in Takagi's experiment and CO-H2-air turbulent diffusion flame used in Correa's experiment, respectively. In the CE-EDC model, the amount of the major species in the CE-EDC model was in good agreement with the experimental data and computational data by using the EDC model when the reaction rates of those species were estimated using the ED model. However, the amount of radical species was not in agreement because the ED model cannot compute the reaction rates of the radical species. In contrast, the amounts of both major and radical species in the CE-EDC model were in good agreement with the reference data when the reaction rates of the species were calculated using the EDC model. Using the developed CE-EDC model, the amounts of combustion products can be calculated without using detailed chemical mechanisms; furthermore, the prediction accuracy of designated chemical species can be improved by taking into account the chemical reaction rates. The accuracy of this model is in the same order as that of the EDC model. Therefore, the CE-EDC model can easily calculate the amounts of chemical species and the temperature.