Effect of pressure-dependent detailed hydrogen chemical reaction model on combustion simulation

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This paper deals with the effect of detailed hydrogen chemical reaction models on numerical simulation in combustion science. Detailed chemical reaction model contains several primal elementary reactions, therefore it may show a better agreement with experimental data than an overall one-step reaction model. However, the detailed models are diverse and have different characters each other because a combination of elementary reactions and the coefficients in their Arrhenius terms depend on each model. It means the result of numerical simulation using detailed chemical reaction model relies on the character of the model. From this reason, it is necessary to choose an appropriate reaction model for the simulation of aimed problem.

Pressure-dependent detailed chemical reaction models are desired for detonation phenomenon because it is a combustion with high temperature and pressure. The reaction model, produced by Petersen and Hanson [1], has been used for detonation simulation for a long time. This model (called Petersen-Hanson model) describes detonation phenomenon well. However, several new upgraded models are developed from several institutions in these years. For example, UT-JAXA model [2], which is developed by University of Tokyo and JAXA (Japan Aerospace eXploration Agency), is generated for high temperature and pressure combustion such as rocket engine combustion. Also, a model (called Stanford model [3]) developed by Hanson at Stanford University is expected as more appropriate model for detonation simulation. Those are relatively new so that the evaluations for those models haven't been well established yet.

There is a considerable open question on numerical simulation for detonation that the numerical detonation cell width is much smaller than the experimental one. It may come from the reason that the simulation corresponding to the experimental scale hasn't been performed much yet due to numerical cost.

This study focuses on the evaluation of several detailed chemical reaction models by comparing various combustion characteristics with experiments such as ignition delay time and laminar flame speed (Figures 1 and 2). This paper also shows the reaction model dependency on detonation to compare between detonation cell structures by Petersen-Hanson model and Stanford model.

The goal of this study is to show detonation phenomenon numerically by comparing numerical results with that of real experimental scale.

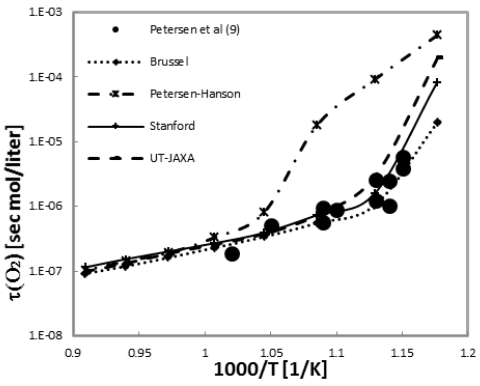

Figure1 Ignition delay time comparison on H2/O2/Ar (97%) mixture, P_0=1atm

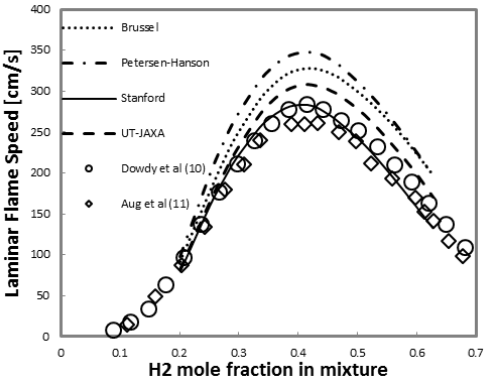

Figure2 Flame speed comparison on H2/Air mixture P_0=1atm, T_0=293K

References

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3. Hong, Z., Davidson, D.F. and Hanson, R.K., Combust. Flame, 158, 2011, pp. 633-644.