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On the optimization routines for calibrating chemistry models for deflagration-to-detonation transition

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The deflagration-to-detonation transition (DDT) is a critical phenomenon in combustion, which occurs in the presence of shock waves, turbulence, and boundary layers. Following the transition to detonation, the velocity of the flame front, temperature, and pressure increase significantly. As such, DDT is a key factor in the design of industrial environments and safety systems [2]. Since detailed chemical reaction mechanisms are often computational prohibitive for practical applications, simplified chemistry models are used to predict DDT in large scale [3]. These models are often parameterized for chemical reaction and diffusive transport and are calibrated to reproduce one-dimensional laminar flame and Zel'dovich-Neumann-Döring (ZND) detonation properties. Previously, various optimization techniques have been employed to calibrate these models, including genetic algorithms and particle swarm optimization. In this study, we compare the performance of four single-step optimization models in predicting DDT in hydrogen-air systems: the genetic algorithm (GA), particle swarm optimization (PSO), GA with the Nelder-Mead simplex method (GA-NM), and the differential evolution (DE) algorithm. Previous studies have shown GA and GA-NM to be effective in predicting DDT [3], while PSO and DE have not been extensively studied. The comparison criteria include the accuracy of the predicted DDT parameters, such as the flame front velocity and DDT distance, as well as the computational efficiency of each optimization method. Preliminary results indicate that DE outperforms the other three optimization methods in terms of computational accuracy and efficiency. The aim of this study is therefore to identify the most effective optimization method for calibrating chemistry models that can predict DDT in hydrogen-air systems and to provide insights into the underlying optimization techniques.

References

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