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Acceleration of Detailed Chemical Reaction Calculations Using GPU and High-Speed ODE Solvers with Application to Ammonia Combustion Furnaces

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In recent years, ammonia combustion has garnered attention as a means of reducing carbon dioxide emissions from industrial furnaces. For practical implementation, it is necessary to reduce NOx emissions, including Fuel NO, in both pure ammonia combustion and co-firing with conventional fossil fuels. While thermal NO is gradually formed in high-temperature regions, Fuel NO in ammonia combustion is rapidly generated in the flame zone, and a portion of it is subsequently reduced through chemical reactions in the post-flame region [1]. Since the balance between the formation and reduction of NO depends on parameters such as species concentrations and temperature in and around the flame, combustion simulations that account for detailed chemical kinetics are effective for accurately predicting Fuel NO. Meanwhile, the volume of a combustion furnace is significantly larger than that of the flame itself, and the time required for the furnace to reach a steady state can be several hours, which is much longer than the timescale of flame reactions. Due to this disparity in timescales, applying steady-state Reynolds-Averaged Navier–Stokes (RANS) simulations makes it feasible to evaluate the steady-state exhaust NO in practical computation time. Although numerical analysis is expected to assist in furnace design, few studies have been reported on the numerical simulation of ammonia combustion in industrial furnaces, mainly due to a lack of experimental data and the difficulty in predicting steady-state behavior using unsteady simulations. The authors have conducted experiments using a 10 kW-scale combustion furnace to evaluate the effects of parameters such as the ammonia co-firing ratio, the primary-to-secondary air ratio in staged combustion, and nozzle configuration on exhaust NO. These studies have revealed that staged combustion can significantly reduce NO emissions compared to single-stage combustion and that the highest NO emissions in staged combustion occur at a co-firing ratio of 50% [2]. To reproduce these experimental results, a numerical solver was developed that incorporates detailed chemical reactions, radiation, and conjugate heat transfer between solid and fluid domains. The Okafor mechanism [3] was used for the chemical kinetics, and to reduce computation time, dynamic load balancing and hybrid parallelization using MPI and OpenMP were implemented for the reaction calculations [4]. Numerical simulations were conducted by varying parameters such as the co-firing ratio and the air distribution ratio, demonstrating that the impact of these parameters on exhaust NO can be accurately predicted [4-5]. On the other hand, further acceleration of the computational method is desirable for simulations of practical-scale furnaces with capacities of around 1 MW. In this study, efforts were made to accelerate combustion simulations considering detailed reactions by utilizing GPUs and optimizing the performance of ODE solvers. Additionally, simulations of ammonia combustion furnaces were conducted to evaluate the accuracy and computational efficiency of the proposed method.

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