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Diagnostics of strongly turbulent premixed flames based on direct numerical simulations

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14. ABSTRACT

The objective of the proposed research is to understand the structure and propagation mechanisms of strongly turbulent premixed flames relevant to high speed propulsion applications. The objective is achieved through computational diagnostics of limit flame phenomena, including local ignition and extinction, and other critical flame features, such as premixed reaction fronts and the associated propagation speed, by using the chemical explosive mode analysis (CEMA) on turbulent flames simulated with direct numerical simulations (DNS). Progress has been made in the following tasks during the reporting period (no cost extension): 1) Developed and validated the deeply reduced kinetic model for JP10 specific to extinction problems based on HyChem, 2) Systematic generation and solution of reactor network models (RNM) based on computational fluid dynamics (CFD) results, and 3) Investigation of chemical kinetic uncertainties propagating in turbulent flames based on 2-D DNS.

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DIAGNOSTICS OF STRONGLY TURBULENT PREMIXED FLAMES BASED ON DIRECT NUMERICAL SIMULATIONS

(AFOSR Grant No. FA9550-15-1-0496)

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SUMMARY/OVERVIEW

The objective of the proposed research is to understand the structure and propagation mechanisms of strongly turbulent premixed flames relevant to high speed propulsion applications. The objective is achieved through computational diagnostics of limit flame phenomena, including local ignition and extinction, and other critical flame features, such as premixed reaction fronts and the associated propagation speed, by using the chemical explosive mode analysis (CEMA) on turbulent flames simulated with direct numerical simulations (DNS). Progress has been made in the following tasks during the reporting period (no cost extension): 1) Developed and validated the deeply reduced kinetic model for JP10 specific to extinction problems based on HyChem, 2) Systematic generation and solution of reactor network models (RNM) based on computational fluid dynamics (CFD) results, and 3) Investigation of chemical kinetic uncertainties propagating in turbulent flames based on 2-D DNS.

TECHNICAL DISCUSSION

1. Reduced JP-10 model specific to extinction problems

In the previous year, a detailed HyChem model for JP-10 including 120-species was systematically reduced, resulting in comprehensive 40-/31-species skeletal/reduced models, applicable for both ignition and extinction problems. Even smaller reduced model can be possibly obtained if only high-temperature strongly burning or near-extinction applications are of interest due to the existence of strong radical pool at high-temperature flame conditions. In such cases, auto-ignition chemistry becomes less important to the flames, such that more species can be assumed to be in quasi-steady state (QSS).

To demonstrate this point, Fig. 1.1 shows the timescale-based reduction curves for two different sampling ranges based on the 40-species skeletal model. Ignition and extinction denote the reaction states obtained from the auto-ignition and perfectly stirred reactor (PSR) solutions, respectively. For the threshold value of ~0.1, while 9-species are identified as QSS species when ignition and extinction samples are considered, more species can be further assumed to be in QSS if only the extinction application is of interest. Thus, a 22-species deeply reduced model specific for the extinction problems is developed, which consists of 17 fuel-cracking species, and 2 intermediate species (C_2H_2, C_3H_3), and 3 major combustion products (CO, CO_2, and N_2) where H_2O is included in the set of fuel-cracking species.

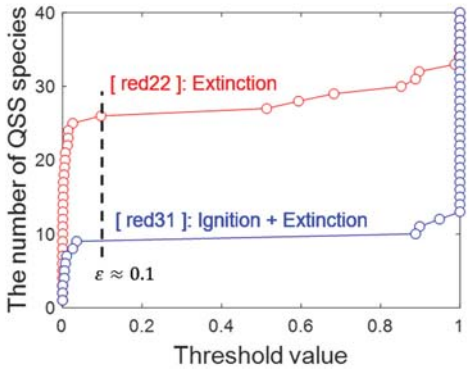

Fig 1.1. Reduction curves for the timescale-based reduction with different sampling ranges.

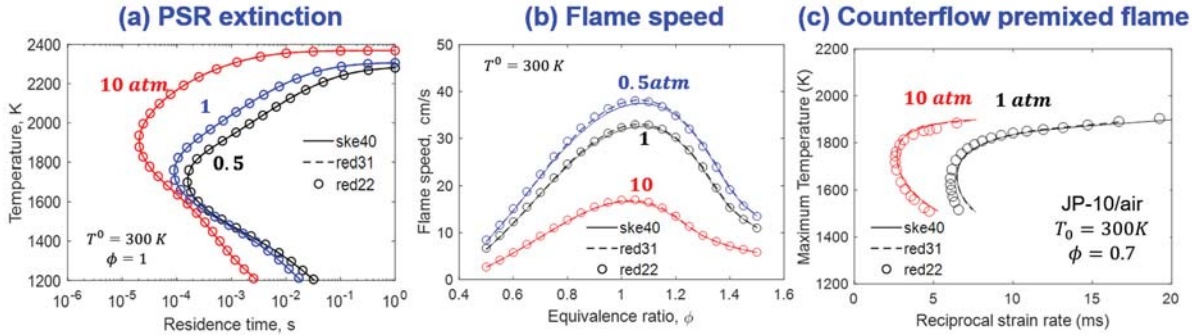

Fig 1.2. Validation of deeply reduced model for PSR extinction (left), laminar flame speed (middle), and counterflow premixed flame extinction (right) for JP-10 mixture, under various operating conditions. Comprehensive skeletal: solid lines, reduced: dashed lines, deeply reduced: symbols.

Fig. 1.2 shows the selected validation results for the deeply reduced 22-species model for PSR extinction (left), laminar flame speed (middle), and counterflow premixed flame extinction (right), compared to the comprehensive skeletal/reduced models. Good agreements are observed for all cases with the worst-case error less than 15% for PSR extinction residence time, ~ 1cm/s for flame speed, and ~ 5% of counterflow premixed flame extinction strain rate. Similar observations were also made for lean and rich cases (ϕ = 0.5 – 1.5).

2. Systematic generation and solution of reactor network models (RNM)

2.1 RNM generation and solvation for Sandia Flame D

Reactor network model (RNM) is an computationally efficient method to incorporate the effects of detailed finite-rate chemistry in studying non-homogenous flows, and has been employed for prediction of pollutant emissions (NO, CO, and soot etc.). In the reporting period, a systematic approach is developed to generate RNM from CFD data through grouping cells that feature similar reaction states. The RNM is then solved efficiently based on analytic and sparse Jacobian techniques such that a large network with hundreds of reactors can be readily solved. Such complex RNM can be used to investigate the responses of a flame to key inlet parameters.

A 161-reactor RNM is automatically generated based on Sandia Flame D simulated by using OpenFOAM and RANS. Fig. 2.1 shows the temperature field as a function of the normalized local equivalence ratio colored by the magnitude of the eigenvalue of the chemical explosive mode

(CEM) of the CFD results. Each dot represents a control volume in the CFD data.

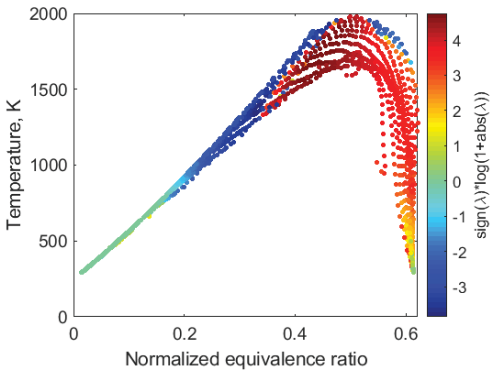

Fig 2.1. Scatter of temperature vs. equivalence ratio in the Sandia Flame D data, Color indicates the CEM eigenvalue.

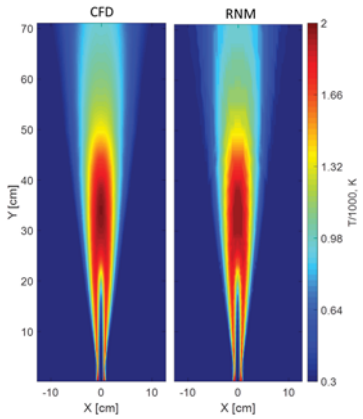

Fig 2.2. Comparison of temperature contours from CFD (left) and RNM (right).

The RNM was constructed by aggregating the control volumes based on temperature, equivalence ratio and eigenvalue of the CEM. Each reactor in the RNM is a PSR. The mass flow between each pair of reactors is the summation of the convention and the turbulent diffusion fluxes. The reactor temperature is the average temperature of all the control volumes assigned to the reactor. In Fig. 2.2, and is fixed while the species concentrations are solved.

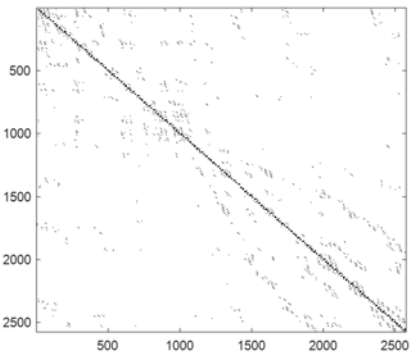

Fig 2.3. Sparse pattern of the Jacobian matrix

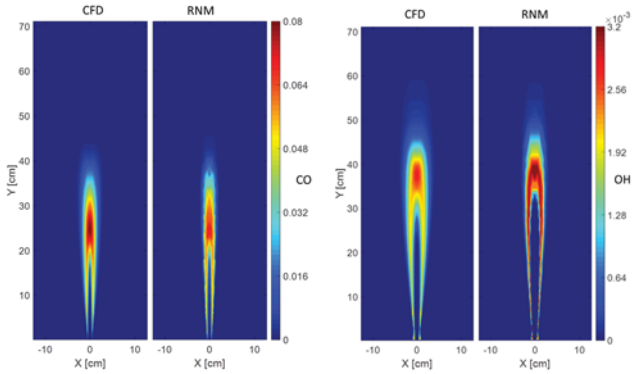

Fig 2.4. Comparison of the CO and OH contours from the CFD (left panels) and RNM (right panels)

The RNM is solved by the TWOPNT solver developed by the Sandia National Lab to ensure the robustness and computational efficiency. The Jacobian matrix of the RNM is highly sparse due to the sparse connection of the PSRs in the RNM and the sparse pattern of the Jacobian is displayed in Fig. 2.3. A sparse matrix package MA48 is employed together with the Newton solver. The RNM is validated against the CFD results for selected species as shown in Fig. 2.4.

3. Propagation of uncertainties in chemical kinetics based on DNS data

A systematic approach to investigating the propagation of uncertain chemical kinetic parameters are studied based on 3-D DNS data of spherical flame kernel of real fuel (JP-8) in homogeneous isotropic turbulence. 2-D Snapshots of the cross-section obtained from 3D simulations are visualized in Fig. 3.1. The snapshot is employed to measure the importance of each reaction to the overall reaction flux. By perturbing 99 reactions simultaneously, the top 19 reactions are selected from the ranked sensitivity spectra and investigated by performing a large

collection of 2-D Monte Carlo DNS simulation with two different sets of perturbed rate sets, SET120 and SET400.

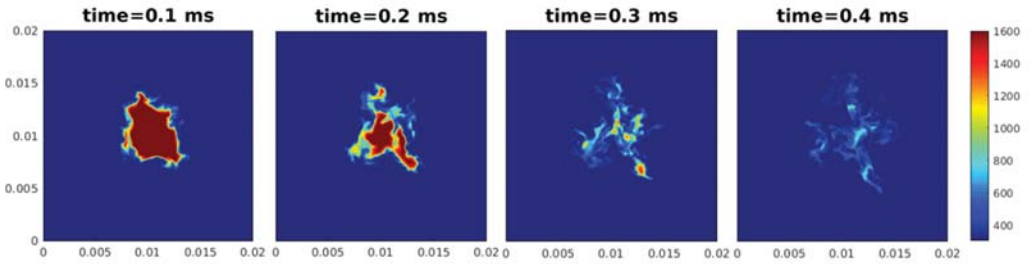

Fig 3.1. Isocontours of instantaneous temperature across the central plane from the 3-D simulation in four time instances.

Heat release rate (HRR) is directly related to the fuel oxidation process and the integrated HRR is closely related to turbulent burning rates, such that its response to the uncertain kinetic parameter is of primary interest. The temporal evolution of integrated HRR over the entire domain is shown in Fig. 3.2. Two distinct (upper and lower) bounds of the solutions are identified, where the upper bound solution shows a slower decrease in the integrated HRR than the lower bound solution.

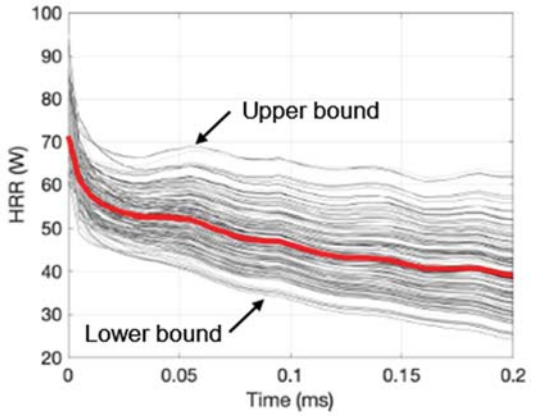

Fig 3.2. Temporal Evolution of integrated heat release rate. Each grey curve denotes results from one simulation using SET120 and the red curve represents the result obtained from the nominal simulation.

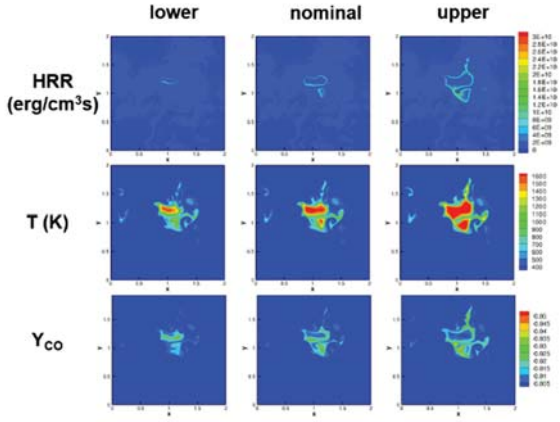

Fig 3.3. Isocontours of HRR, temperature, CO mass fraction for the lower bound, nominal solution, and the upper bound.

Fig. 3.3 shows the HRR, temperature, and CO mass fraction, extracted from the final snapshot of the cases corresponding to the upper bound, lower bound and nominal cases, starting from the same initial conditions. Qualitatively different spatial distribution and its magnitude are observed for all quantities considered here, such that potential impacts of uncertain kinetic parameters in predictions of flame structures and their evolutions are expected.

To understand the differences in HRR evolution in DNS data, several key flame properties, including the laminar flame speed, ignition delay, and the extinction strain rates of twin-premixed flame, are computed and summarized in Table 1. It is found that the upper bound solution, which shows the more persistent ignition kernel in DNS yields a “faster” oxidation process: the laminar flame speed is faster, the ignition delay is shorter, and extinction strain rate is larger. On the other hand, the lower bound solution, showing the extinguished ignition kernels, exhibits a “slower”

oxidation process, such that the opposite trends are found for all three properties. It is noted that the differences between the perturbed and nominal cases in ignition delay and extinction strain rates are much more prominent than those in laminar flames.

Table 1. Comparison of key combustion properties between perturbed and nominal kinetic models. The laminar flame speed and extinction strain rates are computed at boundary conditions that correspond to the DNS condition (T = 300 K, p = 1 bar, and ϕ = 0.7), while ignition delays are calculated at several initial temperatures, and only results at T = 1200 K are reported as the trends are similar for other temperatures

Case	Flame speed (m/s)	Ignition delay (ms)	Extinction Strain rate (1/s)
nominal	0.228	1.29	197.67
lower	0.181 (−20 %)	4.37 (+239 %)	95.81 (−52 %)
upper	0.274 (+20 %)	0.66 (−49%)	396.50 (+101 %)

It is also found that the integrated HRR is most sensitive to reactions R8 and R32. Similar rate limiting processes are found between the turbulent and laminar conditions, although, for certain reactions, the magnitudes of sensitivity coefficients are notably larger under turbulent conditions due to the enlarged thermochemical space. Overall, the results reveal the enhanced sensitivity of turbulent flame predictions to chemistry uncertainties in comparison to laminar flames.

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