

Analysis of Chemical Structure using CSP applied to Triple Flames of Methane and n-Heptane

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Abstract—Computational Singular Perturbation (CSP) is used to analyze the important chemical and transport processes emphasizing the distinction between slow and fast dynamics in two triple flames of methane and n-heptane. The triple flames are computed in a fuel/air mixing layer and uniform inflow velocity in 2D geometry. CSP is employed to study the mode structure and time scales inside these flames. Important chemical reactions and transport processes are studied for major species and some radicals highlighting the different information obtained from CSP importance indices as compared with reaction flow analysis. Important reaction pathways are identified for various regions in the triple flames enabling the identification of different burning regimes. We also discuss explosive modes, i.e. modes with positive real eigenvalues, found in these flames and discuss their physical/chemical interpretation.

I. INTRODUCTION

Computational Singular Perturbation (CSP) has been successfully applied to reduce chemical reaction mechanisms [2], [3], to the analysis of flame structure [4], [5], as well as, a means to the efficient integration of stiff ODE systems [6], [7].

CSP relies on the existence of a number of dissipative chemical time scales which are much faster than those characteristic of the system's evolution, see e.g. [1]. With CSP the various processes in the model can be distinguished as either fast or slow. The fast processes are quickly equilibrated. The fast time scales become thus exhausted, allowing the slow time scales to characterize the dynamics of the system. In this way, the contribution of the fast and slow reactions to the dynamics and the structure of the flame can be evaluated, by identifying the reactions in equilibrium, the driving reactions, and those unimportant to both the fast and slow dynamics.

In this work, CSP is used to gain an understanding of the physical and chemical processes responsible for the observed flame structure of two idealized edge flames [5], [8]. Edge flames are an important class of flame structures which can be found in many reacting flow configurations of non-premixed and partially-premixed combustion [9], [10]. The idealized edge flame consists of three different reaction zones: a lean and a rich premixed branch and a diffusion flame anchored at the flame tip where the premixed branches meet.

The two edge flames studied here are established in the mixing layer of an incoming flowfield of uniform velocity.

TABLE I
PARAMETERS USED FOR THE TWO EDGE FLAMES.

	methane/air	n-heptane/air
left inflow boundary	air	air
right inflow boundary	pure methane	$\phi = 3.5$
inflow velocity	60 cm/sec	71.7 cm/sec
inflow temperature	300 K	400 K
ambient pressure	1 atm	1 atm
domain size	16 mm x 32 mm	4 mm x 4 mm

A 2D spatial configuration is chosen. The first flame is a non-premixed CH₄/air edge flame, the second one a partially-premixed n-heptane/air flame, see Tab. I. The mixture composition at the inflow boundary is prescribed by an analytical function varying the local equivalence ratio between the values given in Tab. I.

The computational model uses a low Mach number approximation, detailed reaction mechanisms and a mixture-averaged transport model [11]–[13]. The reaction mechanisms used are GRI3.0 [14] for methane and the mechanism of Curran et al. [15] for the heptane flame. The time-dependent computations are carried out until a quasi-steady propagating edge flame is established.

II. RESULTS

The temperature distribution of the methane/air edge flame can be seen in Fig. 1. The figure also shows isocontours of the heat-release rate and three isolines of mixture fraction. The cold mixture flows into the domain from the lower boundary. The flame tip, lean and rich premixed branches can be identified from the heat-release contours. The heat-release in the diffusion flame region is of smaller magnitude and cannot easily be seen in this figure.

A. Mode Structure

The CSP analysis shows the variation of number of exhausted modes across the flame. These modes represent fast processes which are either dormant or cancel each other and thus do not determine the larger-scale evolution of the chemical system. In general, it is found that the largest number of exhausted modes appears in the cold inflow region and around the stoichiometric mixture fraction line in the diffusion flame. The largest number of active modes are found in the premixed flame branches.

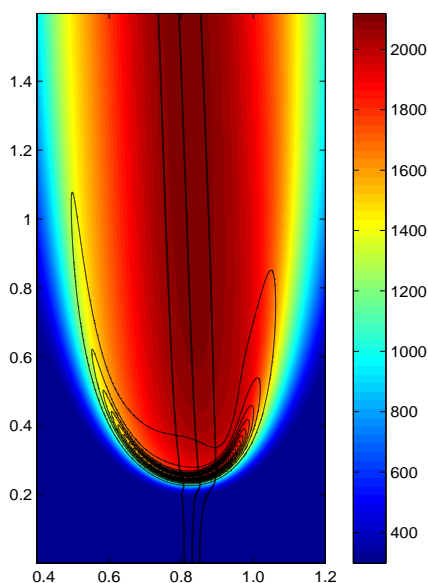


Fig. 1. Temperature profile and contour lines of heat-release rate for the methane/air triple flame. In addition, contours of mixture fraction are shown corresponding to 0.9/1.0/1.1 of the stoichiometric mixture fraction.

The time scales can also be easily identified. The fastest time scale is on the order of 0.7 ns to 2.7 ns varying only slightly across the flame. The time scale of the fastest of the active modes is shown to be large in the inflow region of the flame because there are almost no chemical reactions taking place. In the preheat zone ahead of the premixed flame branches, we find alternating regions of slow and fast driving time scales. The fastest time scales occur again in the reaction zones of the premixed branches, while the diffusion-flame region is characterized by comparably slower time scales.

Participation indices show important transport processes and reactions for each mode. Analyzing the fastest modes helps understand the origin of stiffness of the ODE system aiding in strategies of improving the time-integration of the chemical system. Participation indices of the driving active modes show the importance of transport processes in the preheat zones and show the important chemical pathways.

B. Explosive Modes

In the preheat zone of the premixed flame branches we find chemical modes with positive real eigenvalues, i.e. explosive modes. Figure 2 shows the eigenvalue of the two explosive modes for a cut through the methane/air triple flame along the stoichiometric mixture fraction line. There are two regions of explosive behavior, the slower one at low temperatures below 700 K and the main region in the temperature range between 900 K and 1800 K. In each of these two regions we find two explosive modes (black and red in Fig. 2).

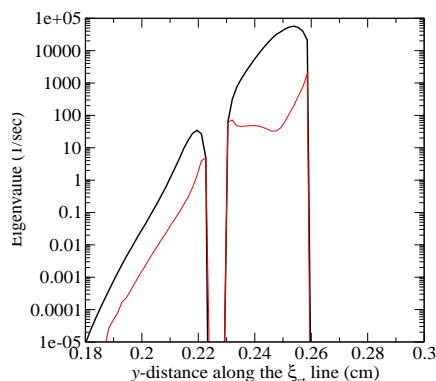


Fig. 2. Eigenvalues of explosive modes for a cut through the methane/air triple flame along the stoichiometric mixture fraction line.

The eigenvector of the fast dominating explosive mode mostly points to temperature, indicating a thermal runaway mechanism behind the explosive behavior. In the main explosive zone, the reaction $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$ is found to have a dominating participation index in the explosive mode. This reaction is an important radical chain branching reaction in methane/air flames.

The participation indices of the explosive modes show also the significance of different species- and energy-transport processes in initiating the chemical activity in these flames.

C. Reaction Networks

A similar analysis as for the methane/air edge flame was carried out for the n-heptane/air flame. Many features are found to be similar between the two flames. In addition, the information contained in the importance indices of species is used to construct reaction networks in different regions of the edge flame to identify the different chemical pathways taken in these regions. This process is the same as used in generating skeletal mechanisms [2], [3]. Starting from a set of target species, a skeletal mechanism is constructed by including reactions and species important for the target species. In this way, new species are added to the target species and the procedure is repeated until no new chemical reactions and species are identified.

One result of this analysis is shown in Fig. 3 for the part of the diffusion flame behind the rich premixed branch. It can be seen that mainly C_2H_2 and CH_3/CH_4 are the species that persist behind the rich branch and constitute the fuel of the diffusion flame.

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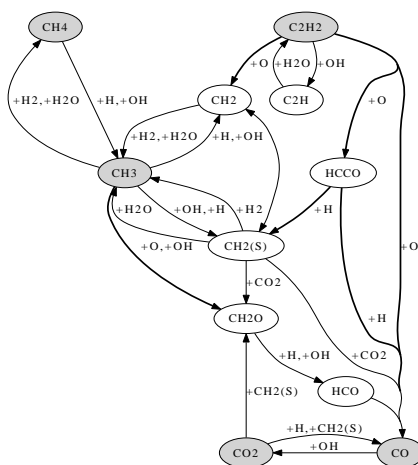


Fig. 3. Reaction network found in the region of the diffusion flame behind the rich premixed branch for the n-heptane/air triple flame. Bold arrows show reaction paths with important contributions to the heat-release rate.

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