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Direct numerical Simulation of turbulent nonpremixed flame extinction by water spray

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Abstract. This paper presents a brief overview of our INCITE 2007 project on the direct numerical simulation of nonpremixed flames subjected to turbulent flows and water spray evaporation. The simulation is a culmination of our recent developments in advanced physical submodels associated with radiative heat transfer and Lagrangian spray dynamics. One of the main objectives is to identify and verify a unified extinction criterion based on the flame weakness factor built on the excess enthalpy variable concept. The results from two-dimensional turbulent ethylene-air flames suggest that the proposed diagnostic tool provides a correct measure of flame weakening. Further work is under way to extend the analysis over a wide range of parametric conditions.

1. Introduction

Recent advances in high-performance computing have enabled the study of three-dimensional, laboratory-scale combustion problems using the direct numerical simulation (DNS) approach [1-3]. The state-of-the-art high-fidelity combustion simulations involve tens of reactive scalar variables, which impart a significant computational overhead in terms of the number of transport equations to be solved as well as the spatial and temporal stiffness arising from the large scale disparities. Furthermore, successful direct simulation of turbulent combustion depends strongly on the fidelity of the embedded physical submodels. The SciDAC project led by a multi-university team [4] has been developing key submodels including thermal radiation based, soot formation, and spray evaporation. A more recent INCITE project [5] has subsequently provided a pilot application of these models to important scientific issues on flame suppression by water spray.

Flame extinction has a significant impact on the performance of non-premixed combustion systems. It determines, in part, the turbulent flame structure and the levels of pollutant emission (NOx, CO, and soot). In engine applications, flame extinction results from the high turbulence intensities associated with the momentum-driven, high-Reynolds number flames and/or the interaction with cold wall surfaces. In fire applications, extinction results from the low combustion intensities associated with the buoyancy-driven, moderate-to-low Reynolds number flames and/or the use of inert gaseous agents or water sprays in fire suppression problems. Laminar diffusion flame theory considers two mechanisms for flame extinction: excessively high values of the rate of fuel-air mixing, that is, insufficient residence times to complete the combustion processes, [6] and excessively low values of the flame temperature, that is, under sluggish combustion conditions that are vulnerable to external cooling. The fast mixing limit is also called kinetic extinction, while the low flame temperature limit is often called radiation extinction [7]. We focus in the following on the kinetic extinction limit in laminar and turbulent flames that are weakened by evaporative cooling from a water spray.

The study of spray-flame interaction has strong scientific and practical relevance, especially in fire suppression technology. Newer designs for water-based fire suppression systems are based on water mist systems [8]. While the conventional sprinkler systems achieve fire suppression by *fuel cooling* and by *flame spread inhibition*, water mist systems achieve suppression by *flame cooling* and have the potential of improved efficiency (reduced water demand) and performance (possible circulation around obstructions and shielded areas). Despite a growing interest in water mist systems, however, a fundamental understanding of the basic physical mechanisms that lead to fire suppression by fine water droplets is still lacking. Key relevant issues include the injection and atomization processes, and overall early liquid water spray dynamics in the vicinity of the injector; the subsequent turbulent dispersion of the water droplets in the fire room and the probability of their transport to the flame location; and the interaction of evaporating water droplets with the turbulent flame, and the resulting decrease in combustion intensity and possible partial/total flame quenching. High-fidelity DNS is well suited to provide valuable information to address these issues.

This paper presents a summary of results from our ongoing investigation of spray-flame interactions. One of the key objectives in this study is to identify a unified extinction criterion that can account for the effects of flame weakening by various heat loss mechanisms. To this end, the concept of the excess enthalpy variable is introduced as a valuable diagnostic that measures deviations from a reference flame conditions resulting from non-adiabatic combustion and non-unity Lewis numbers. The theoretical developments are first evaluated in simulations of spray-flame interactions in the laminar and turbulent counterflow flame simulations.

2. Enthalpy deficit and flame extinction

Following [9], we introduce the excess enthalpy variable, H, that provides a local measure of the relative flame intensity, defined as

$$H = \frac{-(\int_T^{T^{ref}} c_p dT)}{\Delta H_{st}}, \quad (1)$$

where c_p is the heat capacity of the reactive mixture at constant pressure, T the fluid temperature, T_{ref} the local reference temperature (corresponding to the temperature that would be obtained if combustion was adiabatic and occurring at unity Lewis numbers), and ΔH_{st} the heat of combustion (per unit mass of mixture) obtained under stoichiometric, equilibrium chemistry conditions. With this definition, H is a nondimensional quantity that takes on values of order unity: $H = 0$ under adiabatic and unity-Lewis-number conditions; H is negative in the presence of external heat losses (due to radiative heat transfer [10], convective heat transfer to walls [9], or evaporative cooling) and/or negative Lewis number effects; H is positive in the presence of external heat gains and/or positive Lewis number effects. In the present study, H provides a measure of flame weakening due to cooling by evaporating water droplets, combined with possible flame strengthening/weakening due to non-unity Lewis number effects.

Subsequently, non-premixed flame extinction is predicted to occur according to a modified scalar dissipation rate criterion [9,10]; extinction occurs if:

$$\chi_{st} \geq \chi_{st,ext}^{ref} \times \exp(-T_a(\frac{1}{T_{st}} - \frac{1}{T_{st}^{ref}})) \quad (2)$$

where χ_{st} is the scalar dissipation rate at the stoichiometric mixture fraction, $\chi_{st,ext}^{ref}$ is the extinction value of χ_{st} for a reference flame with adiabatic condition and unity Lewis number, T_a is an effective activation temperature, T_{st} is the flame temperature at the stoichiometric mixture fraction, and T_{st}^{ref} is the value of flame temperature for a reference flame at the extinction limit. The RHS of equation (2) is the modified extinction scalar dissipation rate, $\chi_{st,ext}$, accounting for the deviations from adiabatic and/or unity Lewis number combustion. The exponential term in $\chi_{st,ext}$ represents the decrease of the critical value that is expected at lower flame temperatures. In other words, flame quenching is more readily achieved in flame configurations that are weakened by heat losses and/or negative nonunity Lewis number effects.

The extinction criterion may alternatively be cast in the form of a flame weakness factor R [9,10]:

$$R = \left(\frac{\chi_{st}}{\chi_{st,ext}^{ref}}\right) \times \exp\left(T_a\left(\frac{1}{T_{st}} - \frac{1}{T_{st}^{ref}}\right)\right) \qquad (3)$$

such that extinction occurs when $R \geq 1$. Equation (3) can be rewritten as $R \approx (\chi_{st} / \chi_{st,ext}^{ref}) \times \exp(-\beta H_{st})$, where H_{st} is the value of the excess enthalpy variable at the flame and $\beta = T_a (T_{st}^{ref} - T^{\infty}) / (T_{st}^{ref})^2$ is the Zeldovich number with T^{∞} the ambient fluid temperature. The nondimensional activation temperature, T_a, is determined as the sensitivity of the mass burning rate to the adiabatic flame temperature [11]. Note that flame quenching or equivalently large values of the flame weakness factor are promoted by large negative values of the excess enthalpy variable H_{st}, that is, by large values of the flame heat losses.

3. Results and discussion

The current study presents steady counterflow flames that are cooled by fine water droplets that interact with the flame at its vicinity. The flow configuration corresponds to a two-dimensional domain of size 1×2 cm at a strain rate of 440 s^{-1} (40% of the extinction strain-rate). Fuel is injected from the left and oxidizer is injected from the right side boundaries. A reduced reaction mechanism based on directed relation graphs for ethylene-air flame [12] is adopted. Homogeneous turbulence is injected from both vertical boundaries, wrinkling the flame surface. Water droplets are injected at a fixed x-location, but at random y-locations, at the local flow velocity. The droplet injection or loading, defined as a ratio of the latent heat of water droplets injected per second to the integrated flame heat release rate, is set to be 40% of the total flame power, which is expected to weaken the flame significantly enough to cause extinction events [13].

Figure 1 shows an instantaneous image of two-dimensional fields of flame temperature and excess enthalpy variable after the flame-droplet-turbulence interactions have evolved for 40 ms. Droplets are visualized as black dots. The dataset clearly shows variation in the flame thickness due to the action of turbulent eddies. Spray evaporation adds an additional flame weakening effect. The combined turbulence and spray weakening effects are denoted by the excess enthalpy variable isocontours in Figure 1(b), in which two regions of large negative values in the excess enthalpy variable are noticeable: Region A shows a relatively broad flame thickness suggesting that the flame weakening is primarily caused by the spray, while the weakening in Region B is predominantly the action of turbulence straining of the flame.

To further confirm this observation, the spatial variation

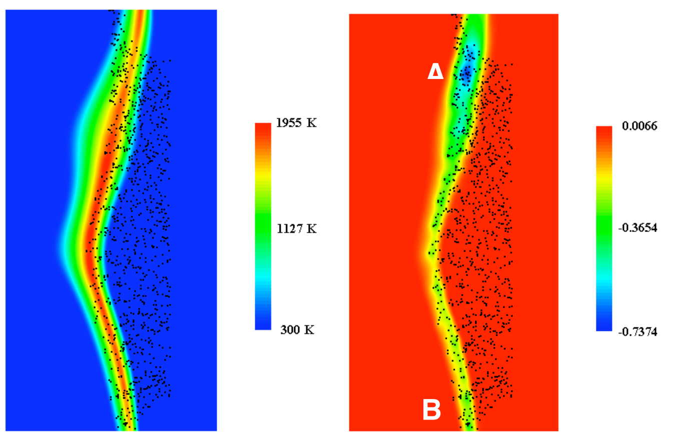

Figure 1. Instantaneous isocontours of (a) temperature and (b) excess enthalpy variable, on which the lagrangian water droplets are overlaid.

along the stoichiometric mixture fraction line (denoted by s) is monitored in terms of temperature, the normalized scalar dissipation rate, $\chi_{st} / \chi_{st,ext}^{ref}$, and the flame weakness factor R defined in equation (3). These are shown in figure 2. The flame temperature is significantly lowered near the zones $1.5 < s < 1.7$ and $0 < s < 0.2$, which correspond to Regions A and B in figure 1, respectively. In the latter (Region B), the large flame weakness factor is primarily due to the enhanced scalar dissipation rate from turbulent eddies, indicating that this is a typical strain-induced flame weakening. On the other hand, flame weakening in Region A is not evidently seen in the scalar dissipation rate, which is actually minimal there, thereby suggesting that the flame weakening is primarily caused by the cooling due to spray evaporation.

As shown in figure 2, the flame diagnosis based on the flame weakness factor appears to provide an unambiguous criterion that accounts for combined effects of flame weakening.

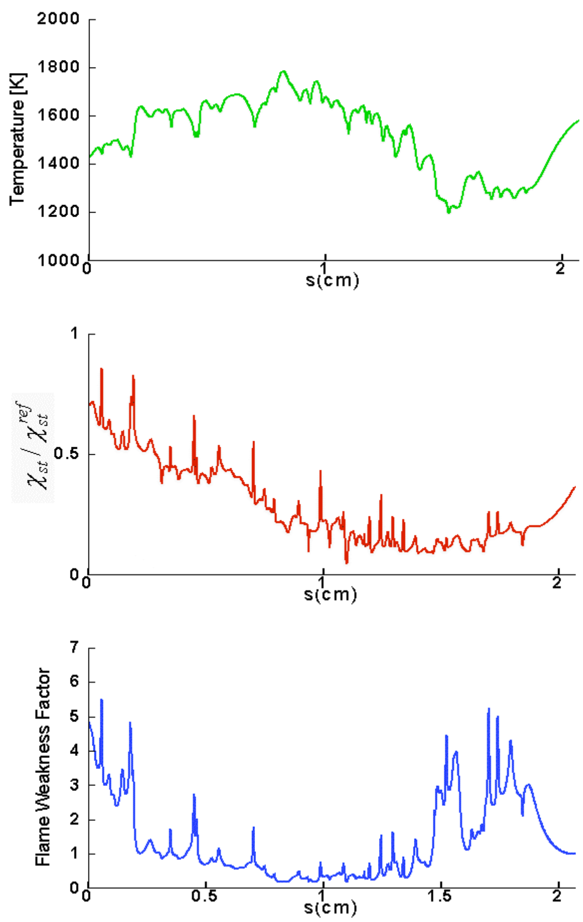

Figure 2. From top to bottom: temperature, normalized scalar dissipation rate, and the flame weakness factor along the stoichiometric line, taken from the data shown in figure 1.

4. Summary and future work

Two-dimensional direct numerical simulations of turbulent counterflow ethylene-air diffusion flames interacting with water spray were conducted. Success in such simulations requires advanced numerical algorithms to deal with strong stiffness arising from detailed chemistry as well as physical submodels associated with radiation and spray dynamics. The main scientific objective of the present study is to identify and verify the unified extinction criterion based on the flame weakness factor built on the excess enthalpy variable concept. Preliminary results are promising but further analysis is needed.

As for future work, more two- and three-dimensional simulations will be undertaken to provide a comprehensive database for parametric studies. Various datasets will be extensively analyzed by using the presented diagnostic tools proposed here, and the results will be synthesized to derive a unified flame weakness metric that accounts for the effects of turbulence and spray evaporation.

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