Local Extinction and Reignition in Nonpremixed Turbulent Jet Flames: A View Using the One-Dimensional Turbulence Model

J. C. Hewson, A. R. Kerstein and J. H. Chen

Combustion Research Facility

Sandia National Laboratory

Livermore, CA 94551-0969, USA

In practical combustors, high-intensity mixing is often desirable in order to minimize combustor volume and also minimize the production of certain pollutants. However, intense mixing may lead to local quenching and potentially a failure to stabilize a flame. The crucial issues are what fractions of the reactive regions are quenched and how rapidly these reacted regions reignite. In this study we apply the recently developed One-Dimensional Turbulence (ODT) model to the study of extinction and reignition in moderately high Reynolds number nonpremixed combustion.

The ODT model

The ODT model is described in detail in a number of recent publications [1–5] and only an overview is provided here. The ODT model has two main components: a one-dimensional evolution equation for the reaction-diffusion terms and a mechanism for turbulent mixing. In this sense, ODT may be viewed as an extension of the unsteady laminar flamelet approach that incorporates the mixing effects of turbulent eddies in the one-dimensional formulation.

To mimic turbulent mixing in a single dimension, a mixing operation is introduced that emulates the effect of an individual turbulent eddy on property profiles along a material line. This operation, denoted the 'triplet map,' is an instantaneous rearrangement of a segment of the one-dimensional domain, corresponding to the zone advected by a given eddy [6]. The triplet map is formulated to have the following desired properties: (1) it wrinkles and folds property profiles, increasing property gradients and the 'area' (points in one dimension) of scalar interfaces, (2) it does not introduce gross artifacts such as property-field discontinuities, and (3) it obeys the relevant conservation laws.

The time sequence of the turbulent mixing operations is determined through the evolution of the velocity field, which is carried on the ODT domain along with any thermochemical state variables. The eddy space/time/size sequence is governed by a stochastic process based on the velocity profiles. Random sampling of eddies is performed, such that the relative frequency of an eddy of given size and location is determined by a measure of shear within the corresponding segment of the 1D domain. The shear is computed from the velocity profiles.

The velocity profiles thus drive the eddies. The eddies, in turn, rearrange the velocity profiles as well as the thermochemical profiles. This two-way coupling of the eddies and the velocity profiles induces complex dynamical behavior within the model, including an eddy cascade that reproduces salient qualitative and quantitative features of the turbulent cascade, in particular the transfer of energy to smaller scales.

The velocity and all state variables evolve by diffusive mixing and chemical reactions (where appropriate) as well as by eddy rearrangements. Flow evolution reduces to a laminar formulation in the absence of eddy events.

Extinction and Reignition

In nonpremixed combustion the rate of combustion is generally driven by the rate of molecular mixing, giving this mode of combustion the moniker 'diffusion flame.' This implies that the chemical reactions are sufficiently fast relative to the molecular mixing process, although no requirements are imposed as to the thinness of any reaction zones. In the present work, reference to flamelets refers to a fragment of the overall turbulent flame, not necessarily thin. If the mixing rates are sufficiently fast, it is found that chemical reactions, notably the heat release, are unable to keep up with the mixing process. The result is that heat losses exceed heat-release rates and the flamelet may be extinguished [7]. Where this occurs, combustion is limited by chemical reaction rates rather than mixing. Within the one-dimensional turbulence model, molecular mixing rates are increased by the advective mixing process, that is by triplet maps that increase the gradients. Reduction of mixing occurs through the molecular mixing process itself.

The rate of molecular mixing may be characterized using a scalar dissipation rate, which itself is defined in terms of a conserved scalar. The conserved scalar selected in nonpremixed combustion is generally the mixture fraction, Z, which represents the mass fraction of an element that originated in the fuel stream; in the present work Bilger's definition is adopted [8]. When the flame structure is referenced to the mixture fraction, the flame is located at a fixed value of the mixture fraction, denoted the stoichiometric mixture fraction, Z_{st}. From the gradient of Z is defined the scalar dissipation rate, $\chi = 2D_T(\nabla Z)^2$, where D_T is the thermal diffusivity. In ODT, $\chi = 2D_T(dZ/dy)^2$ where y is the measure of distance along the ODT domain. When the scalar dissipation rate exceeds a critical value, denoted χ_q, that is dependent on the fuel and other boundary conditions, a flamelet may be extinguished. In turbulent flows, the instantaneous dissipation rate is a rapidly varying quantity characterized by a lognormal distribution.

Following extinction, a flamelet may be reignited by one of two means. First, an edge flame or triple flame may propagate along lines of stoichiometric mixture fraction [9]. However, triple flame propagation is not possible in ODT because it relies on unaligned gradients of the mixture fraction and a progress variable; along the one-dimensional ODT domain all gradients are aligned by definition. The second means of reignition is through interaction with neighboring flamelets; this flame-flame interaction (FFI) is the only possible means of reignition within the ODT model. In FFI, heat transfer normal to the lines of constant mixture fraction leads to reignition of the flamelet. Sripakagorn et al are conducting direct numerical simulations to study the relative importance of each of these means of reignition [10, 11] in another study.

Results

The purpose of the present study is to ascertain the dependence of extinction and reignition (via FFI only) on the instantaneous scalar dissipation rate evolution, considering the effects of both the mean dissipation rate and the Reynolds number on the instantaneous dissipation rate. This is carried out in the context of nonpremixed turbulent $CO/H_2/N_2$ (syngas) flames. Two such flames were studied experimentally [12], and the ODT model has been used to simulate the evolution of reacting and nonreacting scalars in those flames [5]. In the near nozzle region the mixing rates are sufficiently high that localized extinction occurs; farther downstream the mixing rates are reduced and the flame is fully reignited.

The present study considers, using the ODT model, a wider range of global mixing rates and Reynolds numbers than the previous studies. The global mixing rate is varied through the ratio of the nozzle exit velocity to the nozzle exit diameter, while the Reynolds number is a function of their product. In all cases the mean dissipation rates are well below the critical dissipation rate for extinction and extinction only occurs because of fluctuations about the mean.

As would be expected, local extinction of flamelets increases with increasing global mixing rates. For the lower global mixing rates considered, the fraction of extinguished flamelets is roughly 2%. For the higher mixing rates the fraction of extinguished flamelets exceeds 20%. In the latter case, the critical dissipation rate is exceeded for at most 10% of the flamelets at any given instant. This implies a finite time for reignition as might be expected. It is found in the present work that this finite time for reignition by FFI is negatively correlated with the dissipation rate. This implies that larger dissipation rates lead to more rapid reignition as well as more frequent extinction.

The variance of the dissipation rate is also dependent on the Reynolds number, in a manner that has been estimated using a lognormal model [13]. For larger Reynolds numbers at a fixed global mixing rate, it is observed that extinction develops more rapidly during the flame evolution in agreement with the increase in the fraction of instantaneous flamelets for which $\chi_{st} > \chi_q$. Similarly it is observed that the reignition by FFI is also more rapid at larger Reynolds numbers. This implies that the highest excursions about the mean, which are more frequent at higher Reynolds numbers, are relevant to describe both the extinction and FFI reignition processes.

In summary, the results using the ODT model indicate a positive correlation between both (1) the rate of extinction and the probability of large dissipation rates and (2) the rate of reignition by FFI and the probability of large dissipation rates.

The question arises as to whether the FFI mode of reignition or the triple flame/edge flame mode of reignition should be most significant. This question can not be answered in the present study that does not consider triple flames and must await the results of direct numerical simulations. However, simple scaling arguments are proposed here. First, the triple flame must propagate to close a gap caused by the extinction event. In the presence of turbulence there is a tendency for this gap to increase due to flame stretch on the stoichiometric surface; this is easiest to see in flame surface density models where the flame stretch is always a source of flame surface [14]. Because flame stretch tends to bring adjacent flame surfaces together, it is hypothesized that large flame stretch would favor FFI reignition over triple flame closure of extinguished pockets. Correlating locally large flame stretch with locally large dissipation rates necessary for extinction implies that FFI should be the dominant mode of flame reignition where extinction is significant.

Acknowledgments

The authors would like to thank Professor Kosály for stimulating discussions that led to the consideration of the Reynolds number effects. This research is supported by the Division of Chemical Sciences, Office of Basic Energy Sciences, United States Department of Energy.

References

[1] Kerstein, A. R., *J. Fluid Mech.*, 392:277–334 (1999).

[2] Wunsch, S., and Kerstein, A. R., *Phys. Fluids* (2001).

[3] Echekki, T., Kerstein, A. R., Chen, J.-Y., and Dreeben, T. D., *Combust. Flame* (accepted 2000).

[4] Echekki, T., Kerstein, A. R., and Chen, J.-Y., *Combust. Flame* (submitted 2000).

[5] Hewson, J. C., and Kerstein, A. R., *Combust. Theory Modeling* (submitted 2000).

[6] Kerstein, A. R., *J. Fluid Mech.*, 231:361–394 (1991).

[7] Williams, F. A., *Combustion Theory,* Addison-Wesley, Menlo Park, CA, second edition, 1985.

[8] Bilger, R. W., Stärner, S. H., and Kee, R. J., *Combust. Flame*, 80:135–149 (1990).

[9] Im, H., and Chen, J. H., *Combust. Flame* (submitted 2000).

[10] Sripakagorn, P., Kosály, G., and Pitsch, H., *Annual Research Briefs*, Center for Turbulence Research, Stanford University, 2000, pp. 1–12, .

[11] Kosály, G., personal communication, (2000).

[12] Barlow, R. S., Fiechtner, G. J., Carter, C. D., and Chen, J.-Y., *Combust. Flame*, 120:549–569 (2000) Also http://www.ca.sandia.gov/tdf/DataArch/SANDchnWeb/SANDchn.html.

[13] Gurvich, A. S., and Yaglom, A. M., *Phys. Fluids Suppl.*, 10:S59–S65 (1967).

[14] Kalmthout, E. V., and Veynante, D., *Phys. Fluids*, 10(9):2347–2368 (1998).