Flame Propagation Simulations with RFG Model

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A direct numerical approach to solving turbulent mixing and flame propagation is to model the unsteady turbulent flame surface resolved to the finest scales of turbulence. Turbulence modeling can be accomplished using direct numerical simulations (DNS) or a spectral method. This approach can provide insight into some micro-scale phenomena occurring in turbulent flames, which can not be captured in statistical models based on Reynolds averaging. One of such phenomena is the acceleration of flame propagation due to engulfment of unburnt regions. It can be hypothesized that the presence of turbulent velocity fluctuations speeds up flame propagation due to intersections of wrinkled flame surfaces and engulfment of unburnt regions inside the burnt regions. This effect can be qualitatively checked using computer simulations of a turbulent flow-field by spectral method and computing a simplified combustion process in this flow. In this work we use the RFG procedure [2] and a newly developed convection/diffusion solver to test this effect.

Turbulence model The solution for a turbulent flow is given by the following equations (Kraichnan, 1970) [1]:

$$\begin{aligned} v_i(\vec{x},t) = \sqrt{\frac{2}{N}} \sum_{n=1}^{N} [& p_i^n \cos(\tilde{k}_j^n \tilde{x}_j + \omega_n \tilde{t}) \\ & + q_i^n \sin(\tilde{k}_j^n \tilde{x}_j + \omega_n \tilde{t})] \end{aligned} \tag{1}$$

$$\tilde{x}_j = \frac{x_j}{l},\ \tilde{t} = \frac{t}{\tau},\ v' = \frac{l}{\tau},\ \tilde{k}_j^n = k_j^n \frac{v'}{v'_{(j)}} \tag{2}$$

$$p_i^n = \varepsilon_{ijm}\zeta_j^{(n)}k_m^{(n)},\ q_i^n = \varepsilon_{ijm}\xi_j^{(n)}k_m^{(n)} \tag{3}$$
$$\zeta_i^n, \xi_i^n, \omega_n \in N(0,1), k_i^n \in N(0,1/2),$$

where l, τ are the length and time-scales of turbulence, ε_{ijk} is the anti-symmetric permutation tensor, and $N(M,\sigma)$ is a normal distribution with mean M and standard deviation σ. Numbers k_j^n, ω_n represent a sample of n wavenumber vectors and frequencies of the modeled turbulence spectrum

$$E(k) = 16(\frac{2}{\pi})^{1/2}k^4 \exp(-2k^2) \tag{4}$$

A way of generating random flow-field with this method, which represents a simplified spectral technique, is covered more in detail in [2].

Combustion model A 3D convection/diffusion solver based on a cell-centered scheme was developed to solve for the transport of a scalar variable in a turbulent flow field generated by the RFG procedure above. A scalar variable corresponds to a progress variable P of a premixed combustion reaction, and was allowed to change between 0.0 and 1.0. For a qualitative test of the effect of flame-front acceleration due to turbulent velocity fluctuations a simple combustion model was used, where the progress variable in each cell was updated every time-step according to the following criteria: $IF(P > R)P = 1.0$, where R is the ignition limit. In the absence of turbulence (quiescent flow field) the flame propagation velocity was determined entirely by the diffusion rate constant D and in the absence of diffusion, i.e. D=0, the flame front propagation velocity is 0. When the turbulent velocity perturbation were introduced the flame front started propagating, engulfing the unburnt region.

Results In order to isolate the effect of turbulence from that of diffusion, the diffusion coefficient D was set to zero, which corresponds to zero flame propagation velocity in the absence of turbulent fluctuations. An unsteady turbulent field was generated by the RFG model, and the scalar field was governed by convection and a simplified combustion model described above.

Physical parameters used in the model (dimensionless):

1. Diffusion coefficient: D=0.0
2. Ignition limit: R=0.5

3. Correlations of turbulent velocity fluctuations: $\overline{u_i u_j} = \delta_{ij}$.
4. Turbulent time scale: 1.0
5. Turbulent length scale: 1.0
6. Initial distribution of P along the X-axis:
7. P=1.0 for 0¡X¡4
8. P=0.0 for 4¡X¡16

Computational parameters:

1. Grid dimensions: 16 x 16 x 16
2. Spectral sample size: N=1000
3. Time-step: 0.05

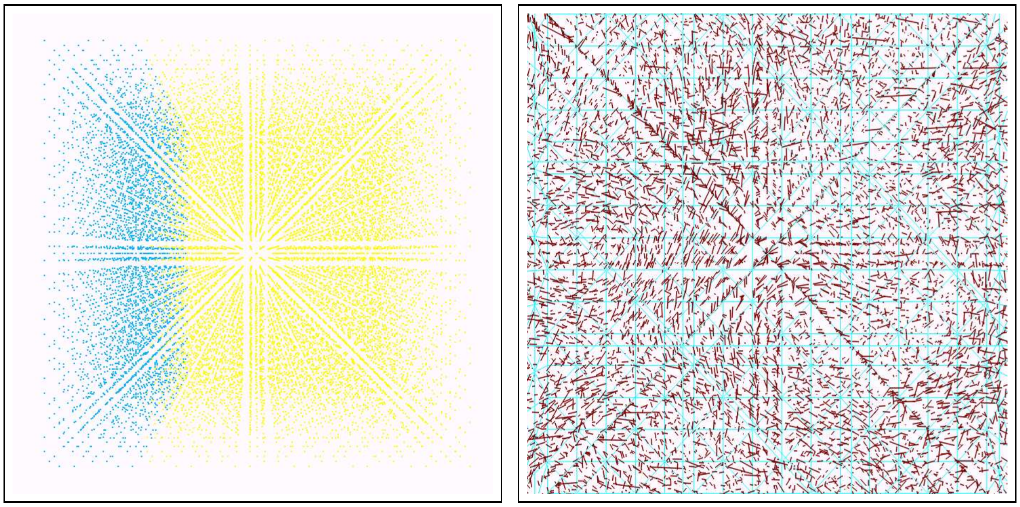
Figures 1,2 show the results of preliminary simulations of flame propagation in a simulated turbulent field. Formation of unburnt and partially burnt pockets inside the burnt region is evident from the figures. An increase of flame propagation velocity from zero to around 1 can be observed.

Conclusions The spectral modeling approach based on RFG algorithm can be used to model micro-mixing in turbulent flames. The results show the increase of flame propagation speed due to turbulent fluctuations. The phenomenon of unburnt pockets entrainment has been captured in the simulations.

References

[1] R.H. Kraichnan. Diffusion by a random velocity field. *Phys. Fluid*, 11:43–62, 1970.

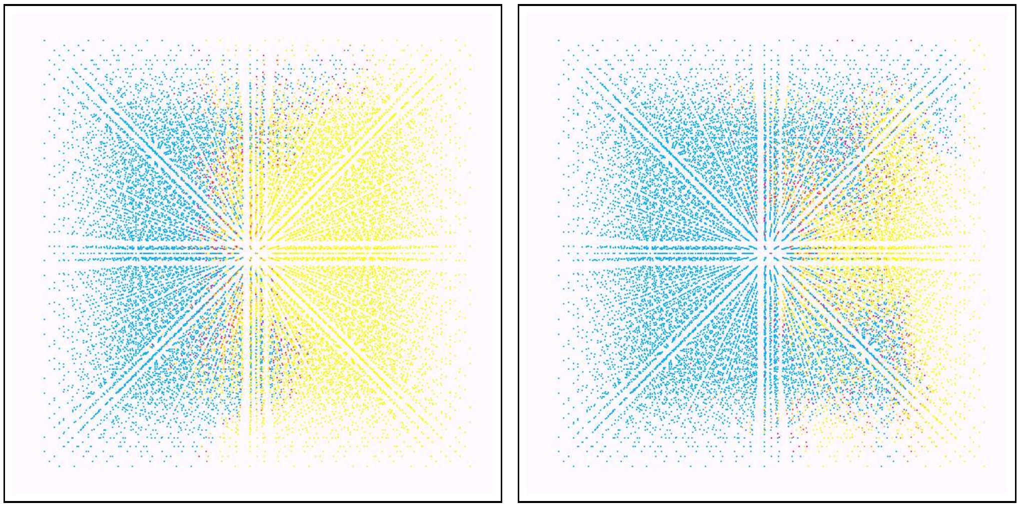
[2] A. Smirnov, S. Shi, and I. Celik. Random flow generation technique for large eddy simulations and particle-dynamics modeling. *Trans. ASME. Journal of Fluids Engineering*, 123:359–371, 2001.



(a) Initial scalar field

(b) Velocity field

Figure 1: Initial scalar field and instantaneous velocity field.



(a) t=3.0

(b) t=6.0

Figure 2: Instantaneous scalar filed at different times.

Each computational cell is represented by a single colored point. Blue color corresponds to fully burnt, yellow - to the unburnt states, and red to the flame surface.