ANALYSIS OF FLAME SURFACE AND TURBULENCE SCALES IN PREMIXED JET FLAMES AT HIGH REYNOLDS NUMBER

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Abstract
A set of Direct Numerical Simulations of turbulent jet flames is performed to investigate the effect of Reynolds number on flame characteristics. The simulations feature finite rate chemistry with 16 species and up to 22 billion grid points. The study covers different aspects of flame-turbulence interaction, including the characterization of the flame surface and the scaling of selected turbulence quantities with respect to variations of the Reynolds number. It is found that the reaction region in the DNS is characterized by a temperature gradient that is close to that of the 1D laminar unstretched flame, while the preheat zone is strongly affected by turbulent transport and the temperature gradient probability density function conforms to an approximate log-normal distribution, typical of turbulent flows. The flame surface has a fractal dimension close to 2.6, in agreement with recent results for low-Damköhler flames. The characteristic length scales of turbulence, i.e., the Kolmogorov and the integral scales, are investigated and the effect of the Reynolds number on these quantities is assessed.

Motivations and goals
The goal of the present investigation is to understand the behavior and the dynamics of turbulent flames at high Reynolds number. This is motivated by the evidence that technical devices, ranging from internal combustion engines for automotive applications to stationary gas turbines for electricity production, operate at high Reynolds numbers. In order to formulate reliable models and to assess their accuracy, detailed DNS data at high Reynolds number are extremely important. On the other hand, it should be recognized that well controlled laboratory experiments and DNS will unlikely be able to achieve the Reynolds number of typical devices of industrial relevance in the near future. This observation motivates the investigation of the trends of key flame properties with respect to variations of the Reynolds number of the flow. From the point of view of basic scientific research, the questions that need to be addressed are:

- How can experimental data and DNS results obtained at low Reynolds number be extrapolated to high Reynolds combustion?

- Does an asymptotic regime of turbulence at high Reynolds number exist in reactive flows? Is it the same of that in incompressible/non-reactive flows?
- Is it possible to approach the asymptotic state of turbulence with DNS in reacting flows?

Description of the DNS database

The flame configuration studied in the present work is a slot jet surrounded by a coflow of burnt gases [1]. This arrangement is similar to piloted flames used in experiments. The simulations feature finite rate chemistry with 16 species and 73 reactions.

Table 1. Parameters of the simulations. Lx, Ly, and Lz indicate the domain size and Nx, Ny, and Nz are the number of discretization points in the three directions. The Karlovitz number is computed in the fully developed region of the flame, in points where the mean temperature is 1800 K, the temperature of maximum heat release rate in the 1D planar unstretched flame.

	R1-K1	R2-K1	R3-K1	R4-K1
Jet Reynolds Number, Re_{jet}	2800	5600	11200	22400
Jet Bulk Velocity, U_b	100 m/s	100 m/s	100 m/s	100 m/s
Slot width, H	0.6 mm	1.2 mm	2.4 mm	4.8 mm
Lx	24 H	24 H	24 H	24 H
Ly	16 H	16 H	16 H	16 H
Lz	8.52 H	4.26 H	4.26 H	4.26 H
Nx	720	1440	2880	5760
Ny	480	960	1920	3840
Nz	256	256	512	1024
Total number of points	88 Million	350 Million	2.8 Billion	22 Billion
Karlovitz number, Ka	≈ 40-50	≈ 40-50	≈ 40-50	≈ 40-50

The gas phase hydrodynamics are modeled with the reactive, unsteady Navier-Stokes equations in the low Mach number limit [2]. The species obey the ideal gas equation of state and all transport properties are computed with a mixture-average approach. The jet consists of a methane/air mixture with equivalence ratio $\varphi = 0.7$ and temperature T = 800 K. All simulations were performed at 4 atm. Relevant parameters are summarized in Table 1.

The bulk jet velocity is $U_b = 100$ m/s, while the coflow has a uniform velocity of $U_c = 15$ m/s. The jet Reynolds number based on the slot width and the jet bulk velocity $Re_{jet} = U_bH/\nu$ varies between 2800 and 22400. The flow is periodic in the spanwise (z) direction, open boundary conditions are prescribed at the outlet in the streamwise (x) direction and no-slip conditions are imposed at the boundaries in the crosswise (y) direction. The jet and the coflow are separated at the inlet by walls with thickness H/10 and length 2H/3.

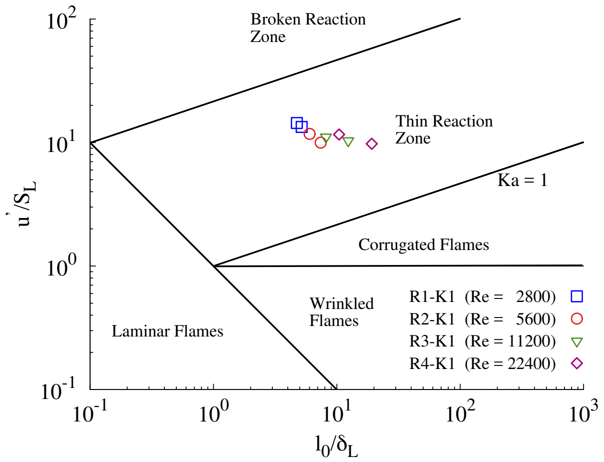

Figure 1. Borghi-Peters diagram for the four flames simulated.

The variation of the Reynolds number is obtained varying the jet slot width H between 0.6 and 4.8 mm, while the jet exit velocity U_b is maintained at 100 m/s. Since the root mean square of velocity fluctuations is expected to be a fraction of $U_{b,}$ (≈10%) independently of the Reynolds number, the simulations will be characterized by an approximately equal turbulence intensity u'.

All the four flames considered are in the Thin Reaction Zone (TRZ) regime as shown in the Borghi-Peters diagram in Fig. 1. The turbulent intensity u' is approximately 10 times the laminar flame speed and the integral scale varies between 5 and 20 times the thickness of a planar 1D freely-propagating unstretched laminar flame with the same fresh-gas conditions of the DNS.

Due to the rather small variation of the Kolmogorov scale among the cases (a detailed analysis of the turbulence length scales is given in the following sections) all the simulations have a Karlovitz number (Ka) between 40 and 50.

Figure 2 shows the mass fraction of oxygen in the four flames at different Reynolds numbers. The range of scales characterizing the fields increases with the Reynolds number. In addition, the figure shows that the length of the flames, measured in terms of the slot width H, decreases as the Reynolds number increases. This is consistent with an increase of the turbulent flame speed due to the increased flame surface area density caused by the larger Reynolds number. The comparison of the 4 fields reveals that the flame-tip dynamics change for the different cases as more and more flame-flame interactions are observed as the Reynolds number increases.

Figure 3 shows the probability density function (PDF) of the temperature gradient in the reaction region (T=1800K) and in the preheat zone (T=900K). It is found that the reaction zone is characterized by a temperature gradient that do not fluctuate significantly with respect to the value observed in the 1D laminar case.

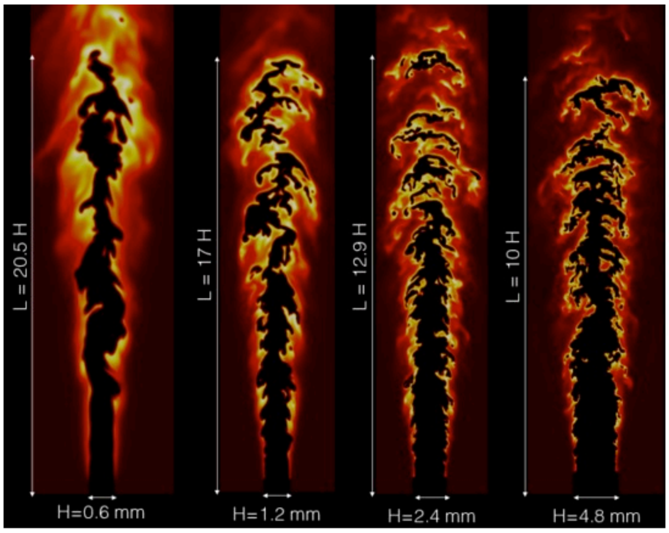

Figure 2. Mass fraction of atomic oxygen in the four flames. The vertical arrows indicate the length of the flames identified by the point on the centerline where the mean temperature is equal to 1800 K corresponding to the maximum heat release rate in a one-dimensional freely propagating plane laminar flame.

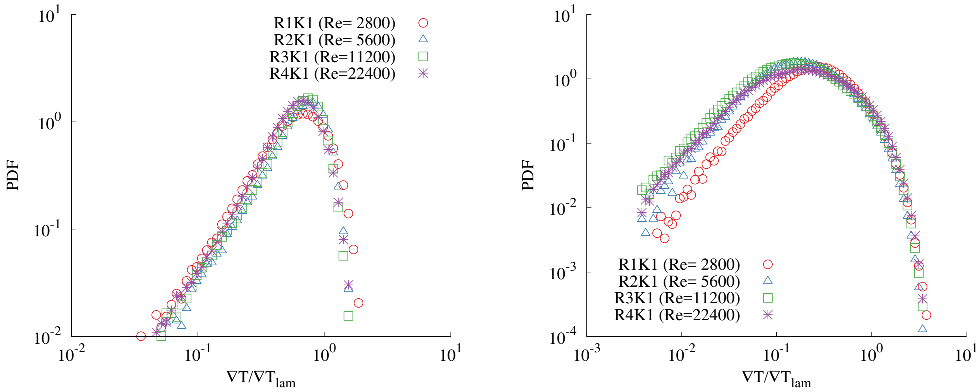

Figure 3. Probability density function of the temperature gradient, normalized with the corresponding gradient in the 1D laminar flame, conditioned on two different temperatures: T=1800K (reaction regions) and T=900K (preheat zone).

On the other hand, the gradient PDF is very broad in the preheat zone and the distribution is close to a log-normal, akin to the typical distribution of gradients in turbulent flows. This is typical of the thin reaction zone regime for which the turbulent fluid dynamics structures are able to affect the preheat zone but not the reaction region. From the analysis of the figure, it is also observed that the gradient PDF tends towards an asymptotic behavior as the Reynolds number increases.

An analysis of the turbulent length scales is shown in Fig. 4. The Kolmogorov (η) and integral scales (L_t) are computed at different streamwise locations both in the preheat and in the reaction regions. The scaling of these quantities with Reynolds number reveals several interesting behavior. The Kolmogorov scale complies with the scaling expected in homogeneous isotropic turbulence ($Re^{1/4}$) in the preheat zone, while a deviation is observed in the reaction zone. The Kolmogorov scale is larger in the reaction layer compared to that in the preheat zone due to the effect of heat release; however, the difference decreases as the Reynolds number increases. Since it is unlikely that η in the reaction layer could be smaller than that in the preheat zone, it is reasonable to speculate that the Kolmogorov scale in the two regions would become the same for even higher Reynolds number. This suggests that the observed effect of the heat release on the smallest scales of turbulence might disappear for very large Reynolds numbers.

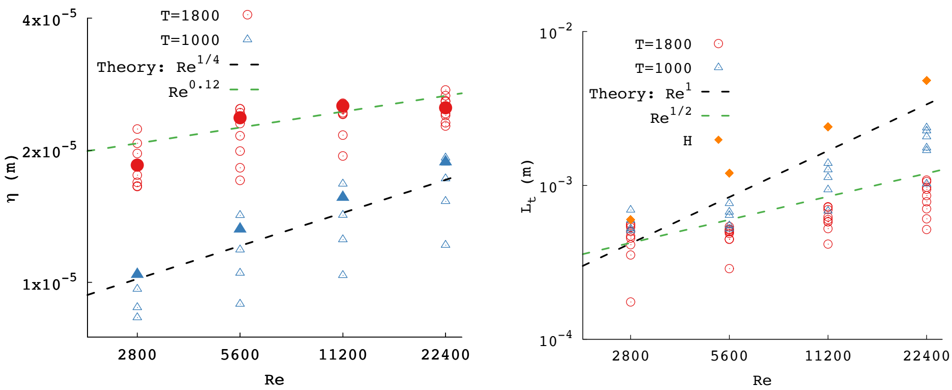

Figure 4. Reynolds number scaling of the characteristic lengths scales of turbulence: Kolmogorov scale normalized with the laminar flame thickness (left) and integral scale (right). The results is shown for the reaction region (open red circles) and for the preheat zone (open blue triangles). The multiple open symbols indicate different streamwise location while the filled symbols show the Kolmogorov scale at half of the flame length. H indicates the jet slot width.

For high Reynolds numbers, the integral scale in the preheat zone tends to the scaling expected for homogeneous isotropic turbulence and become a fraction of the slot jet width, independently of the Reynolds number. From the analysis of the integral scale, it is evident that the deviation from the expected scaling is significant for low Reynolds numbers, pointing out the fact that a sufficiently high Reynolds number is necessary such that the results could be safely considered relevant for real combustion devices.

Figure 5 shows an analysis of the fractal characteristics of the flame surface for the two cases with the highest Reynolds number. The fractal dimension computed with the box counting algorithm is approximately 2.6 for the two flames. This result is in agreement with recent analysis in flames at low Damköhler number [3]. In addition to the relevance for Large Eddy Simulation models, the analysis of the fractal characteristic of flames provide an alternative way, with respect to spectra, for the investigation of the inertial range of turbulence in premixed combustion. From the analysis of the compensated plot shown in Fig 5, it is found that the fractal scaling is observed in a very wide range of scales and up to values that are much larger that the integral scale (shown in Fig. 4).

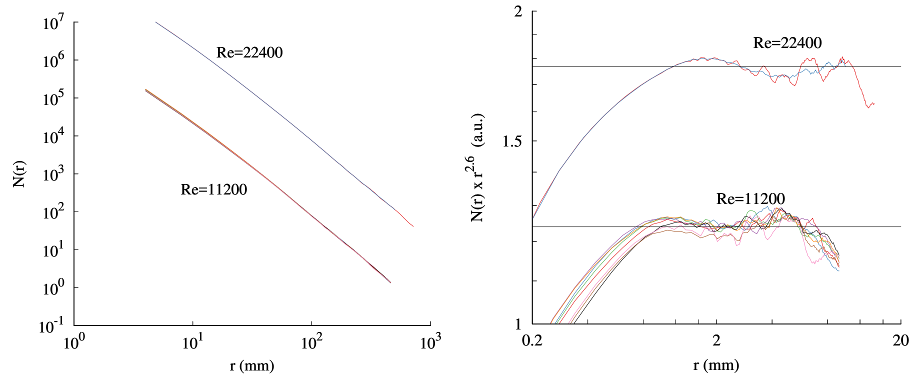

Figure 5. Fractal dimension of the flame. Left: application of the box counting algorithm; number of cubic boxes, N(r), needed to cover the flame surface versus the size, r, of the boxes. The slope in the log-log plot is the fractal dimension. Right: same result compensated with the scaling $r^{2.6}$ to highlight the region where the fractal scaling applies. Multiple lines indicate different time snapshots.

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