# The Role of Flame-Generated Turbulence in the Deflagration-to-Detonation Transition

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## 1 Introduction

Despite decades of research, understanding of the basic physical mechanisms governing the deflagration-to-detonation (DDT) transition still remains largely elusive. Fundamentally, detonation ignition through DDT requires two basic ingredients. First, the flame must be significantly accelerated from the typical highly subsonic speeds characteristic of laminar combustion regimes, and sufficiently large overpressures must be formed in the system. Second, once strong shocks are formed, actual detonation ignition must take place. Countless open questions of fundamental nature remain concerning both of these aspects of DDT. In fact, an extreme multi-scale, multi- physics nature of this process arguably make DDT one of the ”Grand Challenge” problems of classical physics, and any meaningful advances toward its conclusive resolution would require revolutionary breakthroughs in experiments, theory, and numerical modeling.

Conceptually, the problem of DDT can be subdivided into three broad categories based on the type of the physical setting, in which detonation ignition occurs - confined, semi-confined, and unconfined. The first category is arguably best studied, both experimentally and theoretically, and best understood. Experimentally, it is typically realized in the form of either completely closed systems or semi-closed channels with obstacles [1]. Flow confinement in such systems provides a natural mechanism for flame acceleration, which is further assisted by the flow interaction with obstacles. This leads to the formation of strong shocks. Those reflect from obstacles forming hot spots, in which detonation ignition can occur via the gradient mechanism.

Semi-confined systems, an example of which could be an unobstructed channel [4, 5], introduce the next level of complications. While the presence of partial flow confinement still provides a driver for flame acceleration, in the absence of obstacles this process is far less efficient. Consequently, an additional actor historically has been brought to the stage - turbulence. The first question here concerns the source of turbulence, with boundary layers being viewed to act as such a source predominantly, or even exclusively [1]. While there is no doubt that boundary-layer turbulence is present in the semi-confined systems and that it plays an important role, quantitatively such turbulence remains poorly studied. Furthermore, it is not clear if boundary layers are indeed the only source of turbulence in the flame. Finally, the process of actual

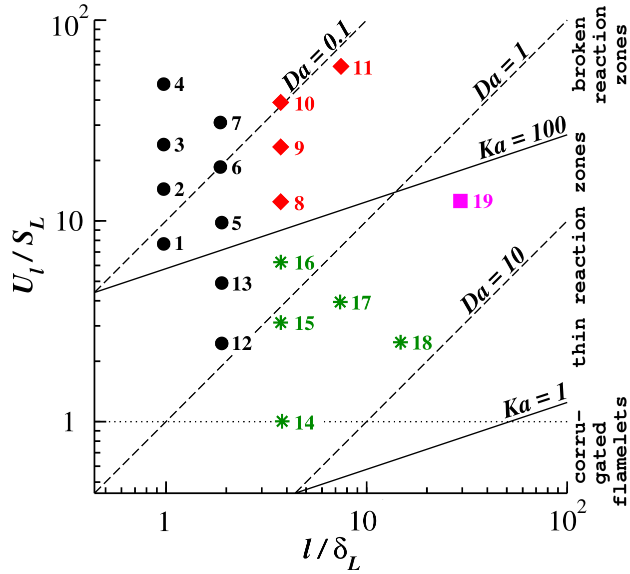


Figure 1: Traditional combustion regime diagram for stoichiometric $CH_4$-air-like (case 11) and $H_2$-air-like flames (all other cases) (cf. Fig. 1 in [2]). Red diamonds mark simulations, in which spontaneous DDT was observed [2], while black circles and green stars represent calculations, in which turbulent flames were found to be, respectively, either quasi-stable [2] or pulsatingly unstable periodically producing pressure waves [3]. Case 19 represents the calculation presented here.

detonation ignition in the semi-confined settings is significantly more enigmatic as it remains largely unclear where the origin of the nascent detonation is typically located (at the wall, inside the flame, immediately ahead of it in the compressed region, etc.) [4] and how the actual ignition occurs - through a spontaneous reaction wave mechanism or through some other process.

Finally, DDT in unconfined systems arguably presents the greatest set of mysteries. Historically, interest in this type of systems was primarily originating in the explosions of astrophysical compact objects, in particular Type Ia supernovae [1]. In the past decade, however, it was rekindled in the chemical combustion community after the infamous Buncefield and Jaipur incidents [6, 7], which emphasized the potential danger of open-air vapor-cloud explosions in industrial settings. In a perfectly unconfined system, absence of flow confinement and boundary layers means that there is no obvious mechanism to provide flame acceleration.

Ultimately, it is reasonable to expect that turbulence is still the only agent capable of accelerating the flame. This immediately raises the question of the turbulence source. In Type Ia supernovae, Rayleigh-Taylor instability has been traditionally invoked as the mechanism of turbulence generation, though on its own it cannot accelerate flames to transonic speeds necessary for detonation ignition, and other additional, more hypothetic, stages of the process must be conjured. These difficulties ultimately brought into question the entire possibility of the existence of DDT in purely unconfined systems.

Therefore, in the context of unconfined systems, the question of possible mechanisms of turbulence generation capable of accelerating the flame sufficiently to form strong pressure waves is central. Furthermore, it is relevant also in the context of more traditional semi-confined settings. In particular, in the latter case, it is important to understand whether boundary layers are indeed the only source of turbulence or whether other processes become activated at various stages of flow evolution. In this contribution, we discuss these ques-

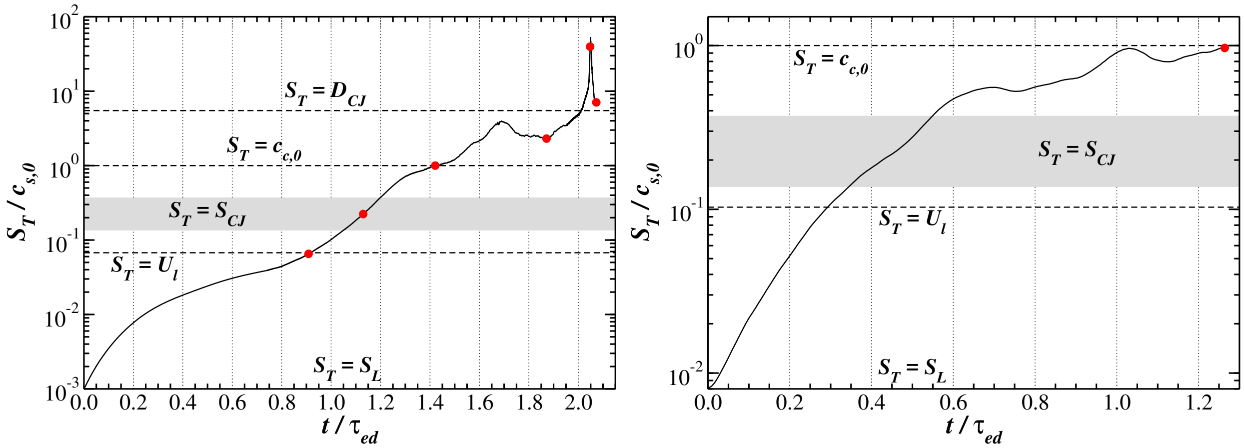


Figure 2: Evolution of the turbulent flame speed, $S_T$, normalized by the sound speed in cold reactants, $c_{s,0}$, in calculation 11 previously presented in Ref. [2] (left panel) and calculation 19 presented here (right panel). Dashed gray region shows the range of values of the CJ deflagration speeds, $S_{CJ}$, based on the sound speed in reactants (lower bound) and products (upper bound). $D_{CJ}$ and $U_l$ are, respectively, the CJ detonation speed in reactants and the nominal integral turbulent velocity in the cold upstream flow.

tions from the point of view of direct numerical simulations (DNS) of the interaction of premixed flames with fast, homogeneous, isotropic turbulence (HIT).

## 2 Results and Discussion

In our previous study [2], we have systematically surveyed a large range of premixed turbulent combustion regimes. In particular, we modeled using DNS the interaction of premixed flames with steadily driven HIT in a rectangular, unconfined domain with open boundaries in the streamwise direction and periodic spanwise boundaries. Results of this survey are summarized in Fig. 1.

In that study, we found that in the presence of sufficiently fast turbulence, turbulent flames exhibited spontaneous transition to a detonation. At some point, turbulent flames would start to accelerate producing a leading planar shock, which preheated and compressed fuel thus further accelerating burning. Resulting runaway process produced strong shock waves, which ultimately led to the formation of a detonation.

It was shown in Ref. [2] that the threshold criterion for the onset of this catastrophic transition was given by the Chapman-Jouguet deflagration speed. Once the turbulent flame speed approached this critical value, the flame would start generating sufficient amounts of energy on its sound crossing time to start the build-up of pressure inside the flame volume in the absence of any external confinement.

For calculation 11, this process is illustrated in Fig. 2(left), which shows the evolution of the normalized turbulent flame speed, $S_T$. The corresponding flame structure and pressure distribution are shown in Fig. 3. Note that this case was not discussed in any detail in Ref. [2]. While all cases shown in Fig. 1 use a simplified single-step kinetics, in case 11 the reaction model was calibrated to reproduce stoichiometric $CH_4$-air flame properties instead of $H_2$-air in all other calculations. As a result, the Mach numbers of both the laminar flame and the initial upstream turbulence were significantly lower than in other cases.

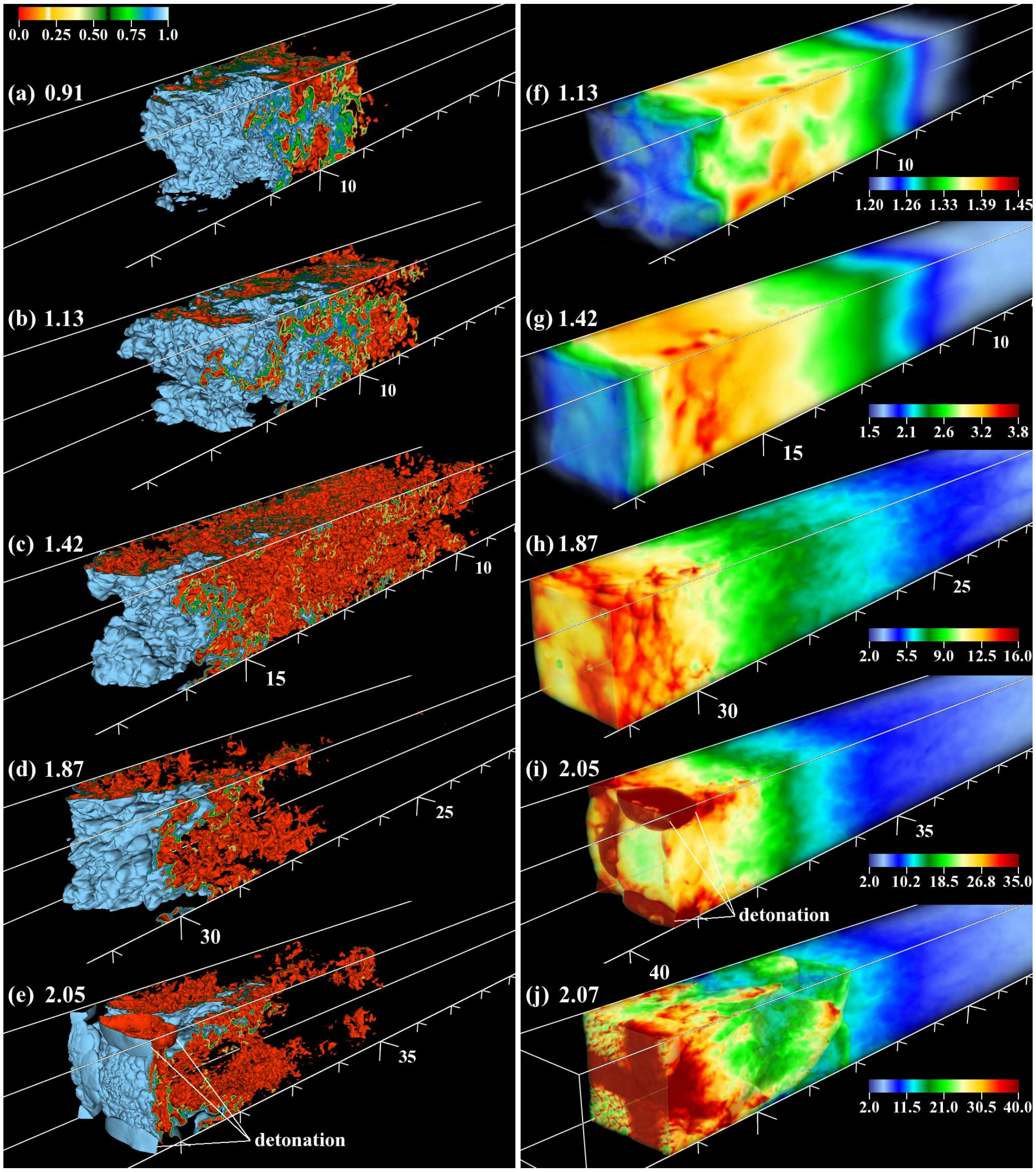


Figure 3: Structure of the turbulent flame and the corresponding pressure distribution during DDT in case 11 (Fig. 1). (a)–(e): isovolume of the fuel mass fraction. (f)–(j): volume rendering of pressure normalized by the initial pressure in the domain (note a different colormap range in each panel). Horizontal axis scale gives the distance from the right boundary of the domain in cm. The time from the start of the simulation is indicated in each panel in units of the large-scale eddy turnover time. Time instants shown are marked with red dots in the left panel of Fig. 2.

Calculation 11 exhibited one peculiar aspect, which again was not discussed in Ref. [2]. In particular, there was an extended period of time approximately between $1.4$ and $1.9\tau_{ed}$, during which the flame was moving in a quasi-steady regime with the displacement speed relative to the upstream fuel of $\approx 1-3$ times the sound speed in reactants, i.e., $\approx 350 - 1000$ m/s. This speed vastly exceeds the characteristic upstream turbulent

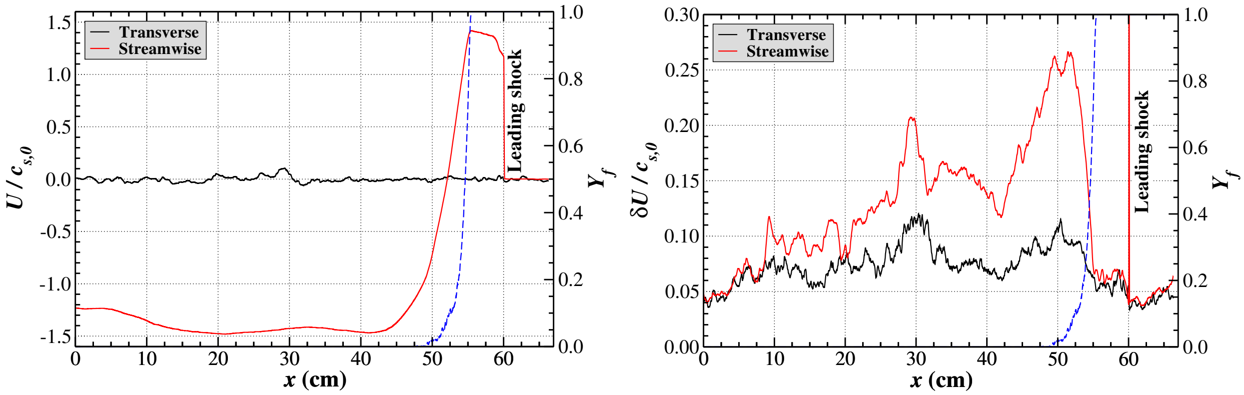


Figure 4: Spanwise- ($y$-$z$-) averaged distributions of the streamwise and transverse velocities, $U_x$ and $U_z$ (left panel), and turbulent velocity fluctuations, $\delta U_x$ and $\delta U_z$ (right panel), in the computational domain along the direction of flame propagation in calculation 19. Turbulent velocity fluctuations in each $y$-$z$ plane are obtained by subtracting the average $U_x$ and $U_z$ in each corresponding plane. Dashed blue line shows the spanwise-averaged distribution of the fuel mass fraction, $Y_f$, indicating the extent of the flame region. All profiles correspond to the time instant marked with a red dot in the righ panel of Fig. 2.

intensity, which was on the order of 30 m/s. Yet as can be seen in Fig. 3 the flame remained turbulent, which raises the question regarding the source of such turbulence. We emphasize that the unconfined computational domain eliminated boundary layers as a possible source of turbulence generation.

In a more recent study [3], we showed that pressure gradients present inside the flame brush provide a powerful source of flame-generated turbulence via the action of the baroclinic torque. This process was analyzed and it was shown that this mechanism results in a range of possible outcomes with DDT being the most extreme one. In particular, at lower turbulent intensities turbulent flames become pulsatingly unstable periodically producing shocks or pressure waves (cases marked with green symbols in Fig. 1).

All calculations $1-18$ (Fig. 1) share one common characteristic. In particular, in all of them turbulence was steadily driven on the largest scale, i.e., on the scale of the domain width. Such large-scale driving is meant to mimic the flux of turbulent kinetic energy in spectral space cascading from larger scales not captured in the calculation. In other words, it assumes that in a real system turbulence would be generated on large scales via some process. In contrast, flame-generated turbulence is superimposed on this process providing the inverse flux of turbulent kinetic energy from small scales, on which it is injected, to larger scales. In this sense, such flame-generated turbulence represents an extreme form of kinetic energy backscatter.

This, however, raises the question of whether such strong flame-generated turbulence can be produced only in the presence of a dominant forward cascade of turbulent kinetic energy from larger scales or whether it can represent a self- sufficient process. As was discussed above, the key issue in unconfined systems is that in them there is no mechanism of large-scale turbulence generation. Furthermore, even in semi-confined systems, boundary-layer-driven turbulence may not envelope the entire turbulent flame brush (at least during the earlier stages of the evolution).

In order to address this question, recently we performed a systematic analysis of flame-generated turbulence in the presence of decaying, rather than driven, upstream turbulence. Calculation 19 (Fig. 1) provides an illustration of the obtained results. This calculation uses the same single- step, $H_2$-air-like reaction model as in other cases $1-10$ and $12-18$. HIT was initially prepared in an unconfined domain, however in contrast to prior calculations, turbulence driving was disabled at the moment when a planar laminar flame was initialized in the domain. Subsequent evolution of $S_T$ is shown in the right panel of Fig. 2. Note that this calculation used a very large domain with size $1,024^2 \times 16,384$.

Fig. 2 shows that in this case, similar to case 11, the flame also underwent rapid acceleration becoming transonic within approximately one eddy turnover time. Fig. 4 shows the spanwise-averaged distributions along the domain of the streamwise and transverse velocities and turbulent velocity fluctuations in the domain. It can be seen that the flame forms a leading shock $\approx 4$ cm upstream. More importantly, right panel of Fig. 4 shows that while upstream turbulence is relatively weak with characteristic velocities $\sim 10 - 15$ m/s, turbulent fluctuations inside the flame brush are almost 10 times higher reaching $\approx 90 - 95$ m/s. Such turbulence is generated entirely within the flame and it is able to support the high velocity of flame propagation.

## 3 Results and Discussion

In the talk, we will summarize these findings and, in particular, we will discuss the implications of these effects for the DDT in unconfined and semi- confined systems. Furthermore, we will briefly address the question of how these effects can be incorporated into LES models. As was mentioned above, up-scale transport of flame-generated turbulent kinetic energy can be viewed as a strong backscatter, which can significantly modify the turbulent cascade and can produce the net flux of kinetic energy from the subgrid scales. To our knowledge, existing LES models are not capable of capturing this process. We will also comment on the experimental challenges involved in studying this problem.

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