

Distributed Burning in Chemical and Thermonuclear Flames

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1 Motivation

Distributed burning can occur in both thermonuclear and chemical premixed flames, and results when flame propagation is driven by turbulent mixing that is sufficiently intense to dominate species and thermal diffusion. In the chemical premixed flame context, distributed burning can occur in a number of scenarios, including gas turbines, for example, and may provide a possible route to the holy grail of high efficiency with low emissions. In thermonuclear flames in type Ia supernovae (SNeIa), the Reynolds number can be orders of magnitude in excess of 10^{10} , so an understanding of flames in extremely high turbulence is crucial. This paper provides a review of recent work exploring the transition to distributed burning and properties of distributed flames, scaling laws for distributed flames, and outlines the case for deflagration-detonation transition (DDT) in distributed flames in SNeIa.

2 Regimes of turbulent premixed flames

Turbulent premixed flames are typically characterised by Karlovitz and Damköhler numbers, which (neglecting differences in diffusion coefficients [1]), can be written as $Ka^2 = (\tilde{u}^3 l_F)/(s_F^3 l)$ and $Da = (s_F l)/(\tilde{u} l_F)$, where \tilde{u} and l are the turbulent intensity and integral length scale, respectively, and the flame propagation speed s_F and thermal thickness l_F (taken to be defined for freely-propagating flames following [2]). The Damköhler number represents the ratio of chemical and integral length time scales. The Karlovitz number represents the ratio of Kolmogorov and chemical time scales, and can be thought of as a measure of the strength of the turbulence relative to the flame. Karlovitz and Damköhler numbers can be used to distinguish different modes of burning, and represented on a regime diagram, see page 79 of [1]. Importantly, turbulent eddies in the inertial subrange have the same Karlovitz number, which follows from writing $Ka^2 = \varepsilon/\varepsilon_F$, where $\varepsilon = \tilde{u}^3/l$ and $\varepsilon_F = s_F^3/l_F$, and noting that the energy dissipation rate ε is constant through the inertial subrange (and s_F and l_F are constant properties of the fuel).

Distributed burning necessarily occurs at high Karlovitz number, but the critical Karlovitz number Ka_c above which distributed burning can occur is fuel-dependent, and is indicative of when there exist turbulent eddies comparable in size with the reaction zone thickness δ_F that are sufficiently strong enough to interact with the internal flame structure. For order-of-magnitude discussion, the reaction zone thickness

can be considered to be one tenth of the thermal thickness, which leads to the often-used estimate of $Ka_c \approx 100$.

In the chemical flame context, there is an argument that distributed flames cannot exist (see [1] and the references therein). However, in these typically Bunsen flame examples, the flames are subject to large amounts of stretch rather than homogeneous isotropic turbulence, and also entrain cold ambient fluid, which leads to increasingly-important local extinction, ultimately resulting in global extinction. These kinds of flames are fundamentally different to distributed flames; here, this marks the distinction between broken reactions and distributed burning.

The term ‘distributed reaction’ was first used by Summerfield [3, 4], referring to flames where ‘reaction rate laws and transport processes are modified by the presence of turbulence’. Damköhler [5] identified a limiting behaviour referred to as “the small-scale turbulence”, bounded by $l/l_F < 1$, and suggested scaling laws analogous to laminar flames with molecular diffusion replaced by turbulent diffusion. Williams [6] presents both the extinction argument above, and also considers the limiting behaviour of the “well-stirred reactor”, where turbulent mixing is rapid compared with chemistry, thereby causing combustion to occur in a distributed reaction zone, “with heat release occurring more or less homogeneously throughout the turbulent flame brush and with local fluctuations in temperature and composition being small”. Bray [7] refers to the distributed reaction regime where chemical times are long compared with the largest time scales of the turbulent flow, i.e. $Da_L \ll 1$, and suggests this could be the mode of combustion in the rocket exhaust of [8]. Pope & Anand [9] considered “distributed combustion, in which reaction is distributed more uniformly in space and is not necessarily accompanied by steep spatial concentration gradients”, and indicated that it should occur for $l/l_F \ll 1$.

The above references suggest that the limiting behaviour of distributed burning occurs at small Damköhler number or $l/l_F \ll 1$. However, it is important to note that if the flame is embedded within developed turbulence with sufficient Karlovitz number, then the scales $l/l_F \ll 1$ will be present due to the turbulent energy cascade process. Whatever the integral length scale is, turbulent kinetic energy will cascade to length scales comparable with the reaction zone thickness (with constant Karlovitz number throughout the cascade process); provided that Karlovitz number is sufficient to produce a distributed flame, then the origin of the turbulence is essentially incidental. The necessary and sufficient condition for distributed burning is $Ka \gg Ka_c$, irrespective of Da and l/l_F .

3 Transition to distributed burning

The transition to distributed burning was first demonstrated in the thermonuclear context in [10] using a flame-in-a-box configuration in which arbitrary turbulence levels could be maintained using a momentum source term developed and characterised in [11]. Figures 5 and 6 in [10] show a categorically different flame structure when the Karlovitz number is sufficiently high. An immediate observation is that the reaction zone is no longer a thin interface between fuel and products, but more spatially distributed, and the temperature field resembles a turbulent mixing zone, reminiscent of mixing in a Rayleigh-Taylor instability, for example.

The transition to distributed burning was then explored in chemical flame-in-a-box direct numerical simulation (DNS) with detailed chemistry, first in lean premixed hydrogen [12] (see figure 8), then in compared at different Lewis numbers in methane and propane [13]. It was observed that despite the higher Karlovitz number (≈ 410 compared with ≈ 260 in the supernova flame), these chemical flames present transitionally distributed behaviour. The reaction zone appears only slightly broader than a flame at lower Karlovitz number, and there is less broadening of the temperature field, especially on the products side. This highlights the fuel-dependence of the critical Karlovitz number; it is likely due to a

greater ratio of length scales l_F/δ_F in the chemical flames, compounded by a relatively greater influence of viscosity in the chemical flames.

Three other groups have simulated chemical flames-in-a-box at high Karlovitz numbers; Poludnenko *et al.* [14, 15] in stoichiometric hydrogen (under $Le = 1$ conditions and single-step chemistry), Carlsson *et al.* [16, 17] in both lean hydrogen ($Le < 1$) and lean methane ($Le \approx 1$), and Savard *et al.* [18, 19] in lean n-heptane ($Le > 1$). All three groups found that turbulence was able to influence the preheat zone, but was less able to interact with the reaction zone sufficiently to produce a distributed flame. Moreover, [14] concluded that subsonic turbulence would not be able to produce a distributed flame in stoichiometric hydrogen.

All of the studies above [10, 12–19] report that local reaction rates are reduced at high Ka , but global extinction is not observed; in this flame-in-a-box configuration, there is no opportunity to entrain cold surrounding air, and turbulence is insufficient to reduce the reaction rates sufficiently to cause extinction.

Lapointe *et al.* [20] went further and showed that taking into consideration the turbulence conditions at the reaction zone gave a more appropriate Karlovitz number for classifying whether or not a flame lies in the distributed burning regime.

The flame-in-a-box numerical configuration is convenient for exposing flames to essentially arbitrary levels of turbulence, but realising such conditions in the laboratory is challenging. However, there is some experimental evidence of (transitionally) distributed burning, particularly in high-speed piloted lean-to-stoichiometric methane jet flames; see Dunn *et al.* [21], Wabel *et al.* [22], Zhou *et al.* [23], and the references therein. Again, there is clear broadening of the preheat zone, along with some evidence of thickening of the reaction zone, but a truly distributed reaction zone appears somewhat elusive.

It is this author's opinion that there are still few examples of truly distributed chemical flames in the literature, if any; the expansion due to increasing temperature through the preheat zone combined with the corresponding increase in viscosity (and consequently Kolmogorov length scale) simply inhibits the ability of turbulence to interact with the reaction zone sufficiently to produce a distributed flame.

4 Phenomenology of distributed flames

The fundamental difference between distributed burning and flames at lower Karlovitz numbers is turbulence mixing dominates molecular diffusion of species and heat. It was observed in [12] (figure 9) that probability density functions (pdfs) of scalar gradients tended towards an exponential distribution; characteristic of turbulent mixing of a passive scalar.

An interesting consequence of mixing being dominated by turbulence is that every point in the mixing region is essentially a linear combination of pure fuel and pure product; fluid parcels are materially advected by turbulence with almost no differential/preferential transport. This was found to manifest in joint probability density functions (jpdfs) of fuel and temperature, which move away from the profiles of the corresponding unstretched flat laminar flames (which present strong Lewis number dependence) to a profile that is almost linear (see figure 11 in [10], figure 11 in [12], and figure 6 in [13]).

The dominance of turbulent mixing has a particular consequence for distributed chemical flames whereby there is no change in local equivalence ratio (see figure 12 in [12] and figure 4 in [13]). Hydrocarbons and oxygen are materially advected together in packets dominating differential/preferential diffusive effects that otherwise lead to changes in local equivalence ratio; a distributed flame burns effectively as a unity Lewis number flame.

This idea was reinforced by Savard *et al.* [24], who analysed data from [12] to show each flame has an average structure comparable with an unstretched laminar flame with an appropriate effective Lewis number, and that the effective Lewis number tends to unity in the limit of high Karlovitz number.

Chatakonda *et al.* [25] analysed a number of data sets, including distributed flames from [10], and showed that the transition to distributed burning results in a change in fractal dimension from $7/3$ to $8/3$; again characteristic of passive scalar turbulent mixing.

In the supernova context, an interesting consequence of burning in the distributed regime is that the inductive oxygen flame that normally follows the carbon flame becomes mixed by turbulence, resulting in a compound carbon-oxygen flame [26, 27].

5 Scaling laws and λ -flames

For $Ka \gg Ka_c$, turbulent mixing drives flame propagation, resulting in a flame that behaves as a unity Lewis number unstretched laminar flame, with species and thermal diffusion replaced by turbulent diffusion. This new kind of flame has one remaining degree of freedom, which can be written as a turbulent Damköhler number $Da_T = (s_T l) / (\tilde{u} l_T)$; the ratio of turbulent flame time scale and turbulence time scale at the integral length. Since Ka is fixed, $\tilde{u} \sim l^{1/3}$ (ε is a constant), it can easily be shown that $Da_T \sim l^{2/3}$; the one degree of freedom can be thought of equivalently in terms of Damköhler number or integral length scale.

The distributed flame has only two regimes depending on whether Da_T is greater or less than unity. For $Da_T < 1$ an integral length scale turbulent eddy turns over quicker than the flame can burn through a flame thickness; the flame is mixed before it can burn. In this situation, [28] showed that simple scaling laws can be derived for distributed burning can be developed following [5], which predicts a flame speed and width based dimensionally on a diffusion coefficient \mathcal{D} and reaction time scale τ . Since mixing is driven by turbulence a turbulent diffusion seems appropriate; [28] simply combined a turbulent diffusion coefficient $\mathcal{D}_T \sim \tilde{u} l$ with a turbulent flame time scale τ_T , then, in analogy with [5], predicted scaling laws for turbulent flame speed and width of $s_T = (\mathcal{D}_T / \tau_T)^{1/2}$ and $l_T = (\mathcal{D}_T \tau_T)^{1/2}$, respectively. These predictions can be written in terms of Da_T as $s_T = \tilde{u} Da_T^{1/2}$ and $l_T = l Da_T^{-1/2}$. Specifically, for $Da_T < 1$, the turbulent flame speed is slower than the turbulence intensity, and the flame is thicker than the integral length scale. As Da_T increases towards unity (which can be thought of equivalently as moving to larger integral length scales), the turbulent flame speed and width increase, but l_T/l decreases. At $Da_T = 1$, there is a limiting case where $s_T = \tilde{u}$ and $l_T = l$, which [28] referred to as a λ -flame with local turbulent flame width $l_T = l_\lambda$ and local turbulent flame speed $s_T = s_\lambda$, both constants for fixed Ka . Note that for $Da_T \leq 1$, it can be shown that $s_T = s_\lambda Da_T$ and $l_T = l_\lambda Da_T$. Finally, for $Da_T > 1$, the turbulent flame time scale is shorter than the eddy turnover time at the integral length scale; the flame burns faster than it can be mixed. Therefore, the turbulence can no longer broaden or quicken the flame, and only turbulent eddies of size l_λ or smaller can interact with the flame structure; for $Da_T > 1$, the flame burns locally as a λ -flame, and scales larger than l_λ serve only to move the flame around as if it were a normal unstretched laminar flame.

For this model to be predictive, there are two quantities required, the energy dissipation rate ε (equivalent to Ka) and the turbulent nuclear burning time scale τ_T , which can be obtained empirically from a (small-scale) distributed flame simulation of the appropriate fuel; it is expected that τ_T is independent of Ka in the high- Ka limit.

The scaling laws outlined above were investigated in the supernova context in [28] where good agreement was found with theory; see figure 6 in [28] for turbulent flame speeds as a function of Da_T .

6 Potential for DDT from distributed burning in type SNeIa

The focus of the present paper is a review of distributed burning rather than a comprehensive review of the various potential mechanisms for SNeIa, but a brief outline is warranted prior to a discussion of the potential for DDT from a distributed flame. In essence, the problem is identifying a mechanism that produces an elemental composition with a light spectrum that matches observations. A pure detonation produces burns to nickel producing insufficient intermediate elements, whereas a pure deflagration can leave unburned carbon and oxygen, and so the belief is that a DDT takes place [29, 30]. The challenge is establishing how the conditions arise that necessary for a DDT to occur, and is subject to much debate; see [31–38], for example. Other factors include whether the mass of the star is at or below the Chandrasekhar limit (about 1.4 times the mass of our sun), or the possibility of merger events (two stars colliding); such factors are beyond the scope of this paper.

A typical candidate white dwarf with a mass at the Chandrasekhar limit has a radius of ~ 2000 km and a core of radius ~ 1000 km where slow thermonuclear reactions drive convection. This convection is a process that could last for hundreds (perhaps thousands) of years, whereas the explosion is over in a couple of seconds. Full-star simulations of the convective phase [39] suggest that an ignition event occurs a few tens of km away from the centre of the star, but doesn't discount central ignition. A central ignition (e.g. [40]) would lead to a statistically spherical Rayleigh-Taylor unstable flame burning outwards. An off-centre ignition gives rise to a burning buoyant bubble of combustion products that rises rapidly under the action of gravity [41, 42]. Figure 22 in [39] provides a schematic of the structure of a SNIa with estimates of length and velocity scales. One mechanism [43, 44] has shown that when the bubble reaches the surface, a burning gravity current can propagate around the surface of the star, leading to compression and ignition on the opposite side; a gravitationally-confined detonation.

The case for DDT from distributed burning in SNeIa is set out in [45]; the proposed argument is as follows. Simulations conducted using the Linear Eddy Model (LEM) [46] examined turbulent burning regimes as a flame progress through the star. At early stages, the Karlovitz number is small and the Damköhler number large; the local flame structure is unaffected by turbulence other than the creation of flame surface area, enhancing the overall flame speed. As the flame burns through the star, the Karlovitz number increases and the Damköhler number decreases. The flame becomes distributed when $Ka \gg 1$ while the Damköhler number remains greater than unity; burning as a λ -flame, but it is when $Da \approx 1$ that provides the most likely conditions for DDT. Under such conditions, the 1D simulations presented 'ledges', large well-mixed regions of partially-reacted fuel with a favourable reactivity gradient for DDT through the Zel'dovich mechanism [47]; specifically, this large region can burn faster than a sound-crossing time. Favourable conditions occur when the fuel density is approximately 10^7 g/cm³, with a turbulent intensity above 20% of the speed of sound, and an integral length scale around 10 km. It remains an open question whether such conditions can exist, how and where they would occur, such that a distributed flame could transition to detonation.

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