Approaches to modeling thermonuclear flames

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Turbulence-flame interactions of thermonuclear fusion flames occurring in Type Ia Supernovae were studied by means of incompressible DNS with a highly simplified flame description. The flame is treated as a single diffusive scalar field with a non-linear source term. It is characterized by its Prandtl number, $Pr \ll 1$, and laminar flame speed, $S_{\rm L}$. We find that if $S_{\rm L} \geq u'$, where u' is the *rms* amplitude of turbulent velocity fluctuations, the local flame propagation speed does not significantly deviate from $S_{\rm L}$ even in the presence of velocity fluctuations on scales below the laminar flame thickness. This result is interpreted in the context of subgrid-scale modeling of supernova explosions.

1. Introduction

A class of astrophysical explosions, so-called Type Ia Supernovae (SN Ia's), is believed to involve the formation and propagation of thin thermonuclear fusion fronts. These fronts are similar in many ways to premixed chemical flames and are often referred to as "thermonuclear flames". The issues addressed in this work are motivated in the framework of supernova research, but the results obtained apply equally well to premixed chemical flames with low Prandtl numbers and small thermal expansion rates.

Type Ia Supernovae occur at a rate of approximately two per century per galaxy; their observables include optical spectra indicating the compositional structure of the explosion ejecta, the evolution of the total emitted light with time, and, indirectly, their contribution to the isotopic abundances in the solar neighborhood. Owing to their high optical luminosity, reaching the equivalent of approximately ten billion suns at maximum light, SN Ia's can be observed out to very large extragalactical distances. Theoretically, they are associated with thermonuclear explosions of white dwarf stars composed of carbon and oxygen and stabilized against gravitational collapse by the degeneracy pressure of a relativistic electron gas (Arnett 1969). In one scenario which has been proposed to explain these explosions, a white dwarf at the Chandrasekhar mass limit—the maximum equilibrium mass of a star supported by electron degeneracy, $M_{\rm ch} \approx 1.4$ solar masses—accretes matter from a binary companion and eventually becomes gravitationally unstable. Compressional heating of the core region leads to the ignition of thermonuclear fusion reactions that "burn" carbon and oxygen to heavier nuclei. Slowly at first but with increasing

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intensity as cooling by neutrino emission fails to keep up with the nuclear energy release, a thermonuclear runaway begins at the center of the white dwarf. As the core reaches the critical temperature of $T \approx 1.5 \times 10^9$ K (at a density of $\rho \approx 2 - 3 \times 10^9$ g cm^{-3}), the time scale for nuclear energy release drops to $\sim 10^{-12}$ s, giving rise to the formation of a highly localized burning front that propagates outward as either a detonation or a deflagration (Woosley 1990). This marks the beginning of the actual explosion, terminating in the complete disruption of the white dwarf.

Based on the observational evidence of intermediate elements in SN Ia spectra, detonations can be ruled out as the initial mode of propagation, as they would predict the complete incineration of the white dwarf to iron group nuclei. Deflagrations, on the other hand, are hydrodynamically unstable to both flame intrinsic (Landau-Darrieus) and buoyancy-driven (Rayleigh-Taylor, RT) instabilities. While the former is stabilized in the nonlinear regime, the latter produces a growing, fully turbulent RT-mixing region of hot burning products and cold "fuel" separated by the thin thermonuclear flame (for a more detailed discussion of flame instabilities in this context, see, e.g., Niemeyer & Woosley 1997). Driven predominantly by the shear flow surrounding buoyant large-scale bubbles, turbulent velocity fluctuations cascade down to the Kolmogorov scale $l_{\rm k}$, which may, under certain conditions, be smaller than the laminar flame thickness (Section 2).

As the explosion proceeds, the turbulence intensity grows while the flame slows down and thickens as a consequence of the decreasing material density of the expanding star. After some time, small scale turbulence must be expected to significantly alter the flame structure and its local propagation velocity with respect to the laminar solution. On the other hand, most subgrid-scale models for the turbulent thermonuclear flame brush in numerical simulations of supernovae depend crucially on the assumption of a (nearly) laminar flame structure on small scales (Niemeyer & Hillebrandt 1995, Khokhlov 1995). The intent of this work is to present a first approach to study the regions of validity and the possible breakdown of this "thermonuclear flamelet" assumption.

This paper is organized as follows: we shall summarize the most important parameters and dimensional relations of thermonuclear flames and buoyancy-driven turbulence in Section 2, followed by a brief description of the numerical methods employed for this work (Section 3). In Section 4, the results of a series of direct simulations of a highly simplified flame propagating through a turbulent medium are discussed and interpreted in the framework of SN Ia modeling.

2. Flame properties and model formulation

The laminar properties of thermonuclear flames in white dwarfs were investigated in detail by Timmes & Woosley (1992), including all relevant nuclear reactions and microscopic transport mechanisms. The authors found that the laminar flame speed, $S_{\rm L}$, varies between 10^7 and 10^4 cm s^{-1} as the density declines from 3×10^9 to $\sim 10^7$ g cm^{-3}. The thermal flame thickness, δ, grows from 10^{-5} to 1 cm for the same density variation. Microscopic transport is dominated entirely by electrons close to the Fermi energy by virtue of their near-luminal velocity distribution and

large mean-free-paths. As a consequence, ionic diffusion of nuclei is negligibly small compared with heat transport and viscosity. Comparing the latter two, one finds typical values for the Prandtl number of $Pr \approx 10^{-5} \ldots 10^{-4}$ (Nandkumar & Pethick 1984). Further, partial electron degeneracy in the burning products limits the density contrast, $\mu = \Delta\rho/\rho$, between burned and unburned material to very small values, $\mu \approx 0.1 \ldots 0.5$.

To within reasonable accuracy, one may estimate the magnitude of large-scale turbulent velocity fluctuations, $u(L)$, from the rise velocity of buoyant bubbles with diameter L, $u_{\rm rise} \sim (0.5\mu g L)^{1/2}$, where g is the gravitational acceleration. Inserting typical values, $L \approx 10^7$ cm, $g \approx 10^8$ cm s^{-2}, and $\mu \approx 0.3$, one finds $u(L) \approx 10^7$ cm s^{-1}. For a viscosity of $\nu \approx 1$ cm^2 s^{-1} (Nandkumar & Pethick 1984), this yields the integral-scale Reynolds number $Re \approx 10^{14}$ and a characteristic Kolmogorov scale $l_{\rm k} \approx LRe^{-3/4} \approx 10^{-4}$ cm. Hence, it is clear that soon after the onset of the explosion, turbulent eddies are present on scales smaller than the laminar flame thickness. According to this length scale analysis alone, the flamelet assumption cannot be justified.

However, the low Prandtl number of degenerate matter allows a situation in which the eddy turn-over time on the Kolmogorov time scale, $\tau_{\rm k} \sim l_{\rm k}/u(l_{\rm k}) \sim l_{\rm k}^2/\nu$, is larger than the reaction time scale $\tau_{\rm r} \sim \dot{w}^{-1}$, where $\dot{w}$ is the fuel consumption rate (Niemeyer & Kerstein 1997). This is readily seen by setting $\tau_{\rm r}$ equal to the diffusion time scale $\tau_{\rm d} \sim \delta^2/\kappa$ for stationary flames (where κ is the microscopic thermal diffusivity), yielding

$$\frac{\tau_{\rm k}}{\tau_{\rm r}} = Pr^{-1} \left(\frac{l_{\rm k}}{\delta} \right)^2 \quad .$$

Even if the length scale ratio on the *rhs* is less than unity, the *lhs* can be large for a sufficiently small Pr. In this case, small eddies are burned before their motion can appreciably affect the flame structure.

An alternative, Pr-independent criterion for flamelet breakdown has been proposed (Niemeyer & Kerstein 1997), based on the relative importance of eddy diffusivity, $\kappa_{\rm e} \sim u(l)l$, and microscopic heat conductivity on scales $l \leq \delta$. As $\kappa_{\rm e}$ is, in general, a growing function of scale, the condition $\kappa_{\rm e}(\delta) \leq \kappa$ is sufficient and can be invoked to define the flamelet burning regime. Using the relation $S_{\rm L} \sim \delta/\tau_{\rm d}$, one finds the more intuitive formulation $u(\delta) \leq S_{\rm L}$. In other words, the flame structure on scales δ and below is dominated by heat diffusion as long as the characteristic velocity associated with eddies of a length scale the same order as the laminar flame thickness is smaller than the laminar flame speed. If heat diffusion is the only relevant microscopic transport process, the local flame speed is expected to remain comparable to $S_{\rm L}$ despite the presence of eddies within the flame.

In order to be able to efficiently address this question, we make three assumptions that greatly simplify the problem without violating the underlying physics. Firstly, we note that nuclear energy generation is dominated by a single reaction, ^{12}C(^{12}C,^{24}Si), which is a strong function of temperature only ($\dot{w} \sim T^{21}$). Therefore, the flame dynamics can be well approximated by a single, diffusive progress variable

c that is advected by the fluid and coupled to a strongly nonlinear source term that mimics nuclear burning. Second, the small value of μ suggests that dilatation effects do not play a significant role and may be neglected for the purpose of this study. This, together with the small Mach number of turbulent fluctuations on very small scales, justifies the use of the incompressible Navier-Stokes equations. Finally, we assume that the effect of the turbulent cascade from large scales can be adequately modeled by forcing the flow field on the lowest wavenumbers of the simulation.

3. Numerical technique

The code used to simulate the thermonuclear flame used the pseudo-spectral approach where derivatives are taken in Fourier space but non-linear terms are evaluated in real space (see Ruetsch and Maxey, 1991). The diffusive term is evaluated implicitly such that the code provided stable, accurate solutions even for very small Prandtl numbers. All boundary conditions were periodic, and energy was added at every time step to the lowest wavenumbers by solving a Langevin equation as described in Eswaran and Pope (1988a, 1988b). All of the simulations were carried out in a 64^3 domain and were run for several eddy-turnover times so as to obtain statistical stationarity.

As was mentioned in the previous section, the temperature dependence of the main reaction participating in thermonuclear flame is roughly T^{21}. It was found that a source term $\dot{w} = kc^{21}(1-c)$ (where the $(1-c)$ arises from the dependence of the reaction on reactant concentration) produced too narrow a reaction zone to be easily resolved in space in a three-dimensional simulation. Instead, it was decided to use a source term of $\dot{w} = kc^4(1-c)$, which is still strongly non-linear but produces a reaction zone that can be resolved in a practical three-dimensional simulation. One difficulty that arises in using a pseudo-spectral code to simulate premixed combustion is that the scalar field—in this case, the progress variable—must be periodic. This was achieved by separating the scalar field into two components: a uniform gradient in the direction of propagation of the flame was subtracted such that the remaining field was zero at each end of the periodic box in that direction. Thus, where

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = \mathcal{D} \frac{\partial^2 c}{\partial x_i \partial x_i} + \dot{w}$$

is the transport equation for the progress variable with constant properties, if a uniform gradient β in the x_3 direction (the direction of propagation of the flame) is subtracted,

$$c = \beta x_3 + \theta$$

then the transport equation for the periodic fluctuating component θ is:

$$\frac{\partial \theta}{\partial t} + u_i \frac{\partial \theta}{\partial x_i} + \beta u_3 = \mathcal{D} \frac{\partial^2 \theta}{\partial x_i \partial x_i} + \dot{w}.$$

So long as the reaction zone remained relatively thin and did not approach the boundaries, c remained bounded between 0 and 1. In order to keep the reaction

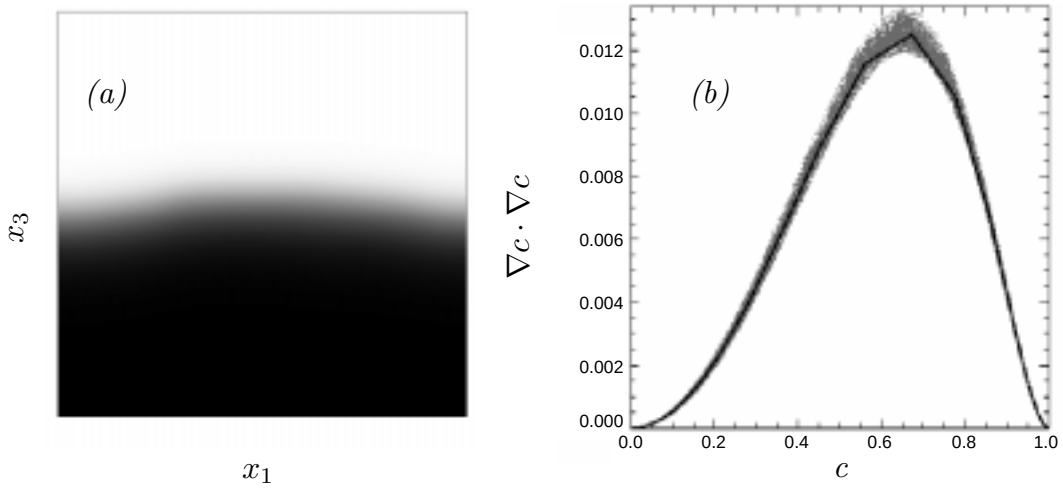

FIGURE 1. a) Snapshot of the scalar field c for $S_{\rm L}/u' = 11.5$ and $Pr = 0.005$ (color scale is linear with $c = 1$ being white and $c = 0$ being black). b) Scalar dissipation rate as a function of reaction progress variable at a fixed time. Superimposed is the line corresponding to the laminar solution.

away from the boundaries, the mean velocity in the direction of propagation was set to the propagation speed of the flame. This propagation speed was determined at each time step from a volume integral of the source term. The need to keep reaction away from the boundaries was found to restrict the simulation to a limited ratio of Prandtl number to k—the flame speed could not be significantly lower than u' or wrinkles in the flame would become too large to be contained in the domain.

3. Discussion of the results

The results of three simulations with varying laminar flame speeds and Prandtl numbers are illustrated in Figs. (1), (2), and (3) (see figure captions for the model parameters). Note that $S_{\rm L}/u'$, with the root-mean-square velocity fluctuation u' dominated in the simulation by eddies on the scale of the laminar flame thickness, corresponds roughly to the parameter $S_{\rm L}/u(\delta)$ employed in Section (2) to describe the validity of the flamelet assumption based on dimensional analysis. Therefore, one may expect noticeable deviations from locally laminar flame propagation for $S_{\rm L}/u' < 1$. Conversely, the dimensional argument predicts that changes of the total burning rate are exclusively due to the growth of the flame surface area by turbulent wrinkling as long as $S_{\rm L}/u' \geq 1$.

We define the turbulent flame speed in terms of the volume integral of the source term, $S_{\rm T} \equiv \Lambda^{-2} \int_V \dot{w} {\rm d}^3\lambda$, where Λ is the grid length. The wrinkled flame surface area, $A_{\rm T}$, is measured by triangular discretization of the $c = 0.5$ isosurface. For the three cases with $S_{\rm L}/u' = 11.5$, 1.15, and 0.95 we find $S_{\rm T}/S_{\rm L}$ ($A_{\rm T}/\Lambda^2$) of 1.008 (1.008), 1.31 (1.27), and 1.51 (1.56), respectively. Hence, to within 5% accuracy the ratio of turbulent and laminar flame speeds is identical to the increase of the flame surface area with respect to the laminar surface, implying that the local flame speed is, on average, equal to $S_{\rm L}$ in all cases.

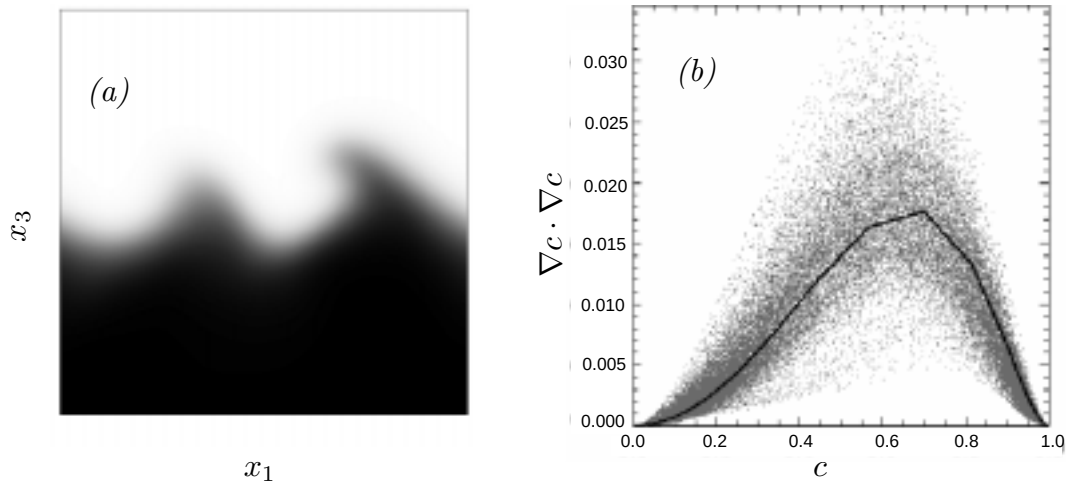

FIGURE 2. a) Snapshot of the scalar field c for $S_{\rm L}/u' = 1.15$ and $Pr = 0.05$ (same color scale as in figure 1a). b) Scalar dissipation rate as a function of reaction progress variable at a fixed time. Superimposed is the line corresponding to the laminar solution.

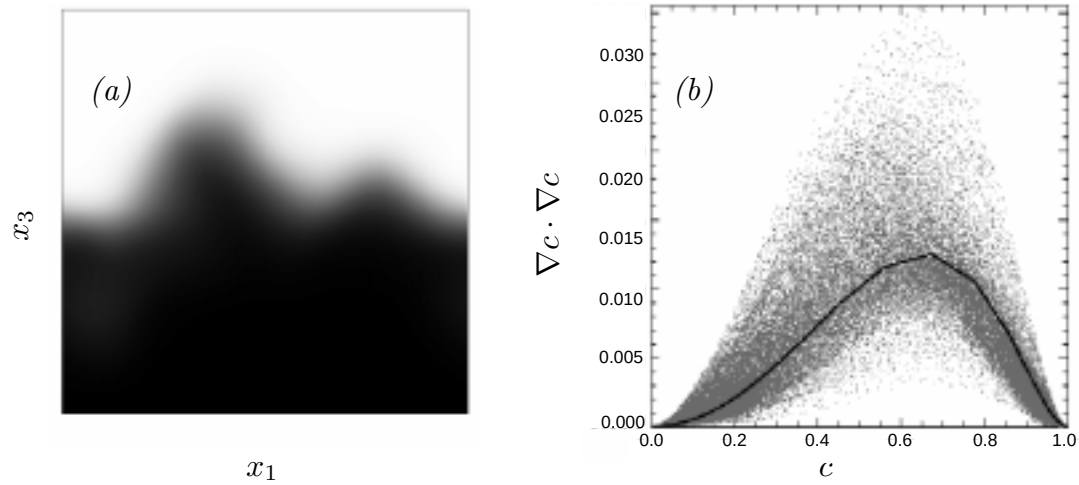

FIGURE 3. a) Snapshot of the scalar field c for $S_{\rm L}/u' = 0.95$ and $Pr = 0.05$ (same color scale as in figure 1a). b) Scalar dissipation rate as a function of reaction progress variable at a fixed time. Superimposed is the line corresponding to the laminar solution.

In conclusion, we have confirmed, within the limitations of the simplified flame description used, that the local propagation speed of turbulent low-Pr premixed flames remains equal to $S_{\rm L}$ if $S_{\rm L} \geq v(\delta)$ even if eddies exist on scales smaller than the flame thickness. For smaller values of $S_{\rm L}/u'$, large scale flame wrinkling forces regions with nonvanishing $\dot{w}$ over the streamwise grid boundaries, violating the requirement of periodicity of the non-linear component of the progress variable. Further investigations using a different numerical technique are needed to observe the breakdown of locally laminar propagation.

In the framework of supernova modeling, this result helps to formulate a subgrid-scale model for the turbulent thermonuclear flame brush in large-scale hydrodynamical simulations. Specifically, it is possible to estimate $S_{\rm L}/v(\delta)$ from the filtered density and velocity strain, using an assumed spectrum for the turbulent velocity cascade. If $S_{\rm L}/v(\delta) \geq 1$, a subgrid-scale model based purely on the surface increase by turbulent wrinkling can be employed (Niemeyer & Hillebrandt 1995). In practice, this is possible for densities above $\sim 10^7$ g cm^{-3} where most of the explosion energy is released. For lower densities (in the late stages of the explosion) relevant for the nucleosynthesis of intermediate mass elements and a possible deflagration-detonation-transition (Niemeyer & Woosley 1997), a more detailed model accounting for small-scale turbulence flame interactions needs to be developed.

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