SMALL-SCALE INTERACTION OF TURBULENCE WITH THERMONUCLEAR FLAMES IN TYPE IA SUPERNOVAE

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ABSTRACT

Microscopic turbulence-flame interactions of thermonuclear fusion flames occurring in Type Ia supernovae were studied by means of incompressible direct numerical simulations with a highly simplified flame description. The flame is treated as a single diffusive scalar field with a nonlinear source term. It is characterized by its Prandtl number, $\Pr \ll 1$, and laminar flame speed, S_{lam} . We find that if $S_{lam} \ge u'$, where u' is the rms amplitude of turbulent velocity fluctuations, the local flame propagation speed does not significantly deviate from S_{lam} 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 and the mechanism for deflagration-detonation transitions.

Subject headings: hydrodynamics - methods: numerical - supernovae: general - turbulence

1. INTRODUCTION

The thermonuclear explosion of a Chandrasekhar-mass C+O white dwarf is presently the most promising candidate to explain the majority of Type Ia supernova (SN Ia) events (Höflich et al. 1996). However, the complex phenomenology of turbulent thermonuclear flames and deflagration-detonation transitions (DDTs) renders a selfconsistent description of the explosion mechanism extremely difficult (Khokhlov 1995; Niemeyer, Hillebrandt, & Woosley 1996; Niemeyer & Woosley 1997). The open questions can be broadly classified as macroscopic ones, pertaining to the global structure of the flame front and the buoyancy-driven production of turbulence, and microscopic ones including turbulence-flame interactions on scales of the flame thickness and preconditioning for DDTs. In this work, the first results of an investigation of the latter will be presented, obtained from direct numerical simulations of a simplified flame model coupled to a threedimensional incompressible turbulent flow.

Based on the observational evidence of intermediatemass elements in SN Ia spectra, detonations can be ruled out as the initial combustion mode after onset of the thermonuclear runaway, 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 buoyancydriven (Rayleigh-Taylor, hereafter 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. 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 (§ 2). This regime is unknown territory for flame modeling; although it has been speculated in the supernova literature that the effect of turbulence on the laminar flame structure is negligible as long as the velocity fluctuations are sufficiently weak, the existence of turbulent eddies on scales smaller than the flame thickness—regardless of their velocity—is in conflict with the definition of the "flamelet regime" in the flamelet theory of turbulent combustion (Peters 1984). No numerical or experimental evidence to confirm and quantify this speculation has been available so far.

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; Niemever et al. 1996). 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. Specifically, a modification of Peters's (1984) flamelet definition suggested by Niemeyer & Kerstein (1997) will be tested.

In addition to the verification of subgrid-scale models, this inquiry is relevant in the context of DDTs which were suggested to occur in SN Ia explosions after an initial turbulent deflagration phase (Khokhlov 1991; Woosley & Weaver 1994). A specific mechanism for DDTs in SN Ia explosions based on strong turbulent straining of the flame front and transition to the distributed burning regime has been proposed (Niemeyer & Woosley 1997; Khokhlor, Oran, & Wheeler 1997). The ratio of laminar flame speed to turbulence velocity on the scale of the flame thickness, $S_{\text{lam}}/u(\delta)$, where δ is the laminar thermal flame thickness, has been suggested as a control parameter indicating the transition to distributed burning when $S_{\text{lam}}/u(\delta) \sim O(1)$ (Niemeyer & Kerstein 1997). One of the main results presented below is that the transition to distributed burning was not observed in the parameter range [$S_{lam}/u(\delta) \ge 0.95$] that we were able to probe.

Thermonuclear burning fronts are similar in many ways to premixed chemical flames. The issues addressed in this work are motivated in the framework of supernova research, but our results apply equally well to premixed chemical flames with low Prandtl numbers and small thermal expansion rates. In order to facilitate numerical computations, we modeled the flame with a single scalar reaction-diffusion equation that is advected in a threedimensional, driven incompressible turbulent flow. The arguments justifying these simplifications are outlined in § 2.

This paper is organized as follows: We shall summarize the most important parameters and dimensional relations of thermonuclear flames and buoyancy-driven turbulence in § 2, followed by a brief description of the numerical methods employed for this work (§ 3). In § 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_{lam} , 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 $Pr = v/\kappa \approx 10^{-5}$ to 10^{-4} , where κ and v are the thermal diffusivity and viscosity, respectively (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, $\mu \approx 0.1-0.5$.

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 $v \approx 1$ cm² s⁻¹ (Nandkumar & Pethick 1984), this yields the integral-scale Reynolds number Re $\approx 10^{14}$ and a characteristic Kolmogorov scale $l_{\rm K} \approx L \times {\rm Re}^{-3/4} \approx 10^{-4}$ 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. In conventional flamelet theory (Peters 1984), the "flamelet regime" is defined based on length-scale arguments alone; that is, if the characteristic length scale of the flame is smaller than the Kolmogorov length, the turbulent flame is said to be in the flamelet regime. Thus, according to conventional flamelet theory, the scaling arguments offered here would clearly indicate that these thermonuclear flames are not in the flamelet regime. Therefore, flamelet-based models such as those used in almost all multidimensional SN Ia simulations would not appear to be applicable for these flames.

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

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

Even if the length scale ratio on the right-hand side is less than unity, the left-hand side 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, $\kappa_e \sim$ u(l)l, and microscopic heat conductivity on scales $l \leq \delta$. As κ_e is, in general, a growing function of scale, the condition $\kappa_e(\delta) \leq \kappa$ is sufficient and can be invoked to define the flamelet burning regime. Using the relation $S_{\text{lam}} \sim \delta/\tau_d$, one finds the more intuitive formulation $u(\delta) \leq S_{\text{lam}}$. 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_{lam} despite the presence of eddies within the flame.

This paper attempts to establish whether or not the newly proposed scaling relationship of Niemeyer & Kerstein is an appropriate definition of the flamelet regime for thermonuclear flames and, more generally, whether or not these thermonuclear flames can be treated as flamelets in numerical simulations. In order to be able to efficiently address this question, we make three assumptions that greatly simplify the problem without violating the underlying physics.

First, we note that nuclear energy generation is dominated by carbon burning which has a very strong dependence on temperature ($\dot{w} \sim T^{21}$). 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 pseudospectral approach, where derivatives are taken in Fourier space but nonlinear terms are evaluated in real space (Ruetsch & 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 & Pope (1988a, 1988b). All of the simulations were carried out in a 64³ domain and were run for several eddy-turnover times so as to obtain statistical stationarity.

As was mentioned in the previous section, the tem-

perature 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 nonlinear but produces a reaction zone that can be resolved in a practical three-dimensional simulation.

One difficulty that arises in using a pseudospectral 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

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

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,

$$c = \beta x_3 + \theta , \qquad (3)$$

then the transport equation for the periodic fluctuating component θ is

$$\frac{\partial \theta}{\partial t} + u_i \frac{\partial \theta}{\partial x_i} + \beta u_3 = \mathscr{D} \frac{\partial^2 \theta}{\partial x_i \partial x_i} + \dot{w} . \tag{4}$$

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 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

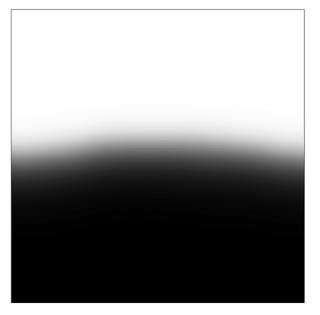
volume integral of the source term. The need to keep the reaction away from the boundaries was found to restrict the simulation to a limited ratio of Prandtl number to k—the flame speed could not be significantly lower than u' or wrinkles in the flame would become too large to be contained in the domain.

4. DISCUSSION OF THE RESULTS

The results of three simulations with varying laminar flame speeds and Prandtl numbers are illustrated in Figures 1-3 (see figure legends for the model parameters). Note that S_{lam}/u' , with the rms velocity fluctuation u' dominated in the simulation by eddies on the scale of the laminar flame thickness, corresponds roughly to the parameter $S_{\text{lam}}/u(\delta)$ employed in § 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 $S_{\text{lam}}/u' < 1$. 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 $S_{\text{lam}}/u' \geq 1$.

We define the turbulent flame speed in terms of the volume integral of the source term, $S_T \equiv \Lambda^{-2} \int_V \dot{w} d^3 \lambda$, where Λ is the grid length. The wrinkled flame surface area, A_T , is measured by triangular discretization of the c = 0.5 isosurface. For the three cases with $S_{\rm lam}/u' = 11.5$, 1.15, and 0.95 we find $S_T/S_{\rm lam}$ (A_T/Λ^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 $S_{\rm lam}$ in all cases.

In conclusion, we confirmed—within the limitations of our simplified flame description—that the local propagation speed of turbulent low-Pr premixed flames remains equal to S_{lam} if $S_{\text{lam}} \ge v(\delta)$, even if eddies exist on scales smaller than the flame thickness. Our results show no indication of a breakdown of the flamelet burning regime in the



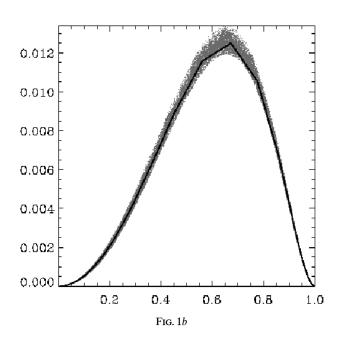


FIG. 1a

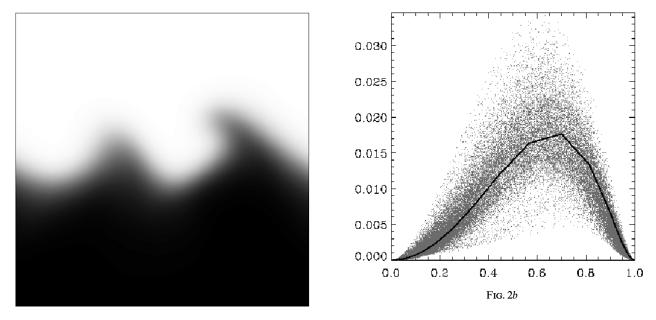




FIG. 2.—(a) Snapshot of the scalar field c for $S_{\text{lam}}/u' = 1.15$ and Pr = 0.05. (b) Scalar dissipation rate $(\nabla c)^2$ as a function of c at a fixed time. Superposed is the line corresponding to the laminar solution.

parameter range $S_{\text{lam}}/v(\delta) \ge 0.95$ that was studied. Lower values of $S_{\text{lam}}/v(\delta)$ were unattainable because large-scale flame wrinkling forced regions with nonvanishing \dot{w} over the streamwise grid boundaries, violating the requirement of periodicity of the nonlinear component of the progress variable. This outcome suggests that the conventional definition of the flamelet regime (Peters 1984) which is based on a length-scale argument alone should be generalized to a timescale-dependent definition in the sense of Niemeyer & Kerstein (1997).

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 $S_{\text{lam}}/v(\delta)$ from the filtered density and velocity strain, using an assumed spectrum for the turbulent velocity cascade. If $S_{\text{lam}}/v(\delta) \ge 1$, a subgrid-scale model based purely on the surface increase by turbulent wrinkling can be employed (Niemeyer & Hill-ebrandt 1995). In practice, this is possible for densities above ~ 10⁷ 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 intermediatemass elements and a possible deflagration-detonation transition (Niemeyer & Woosley 1997), a more detailed model

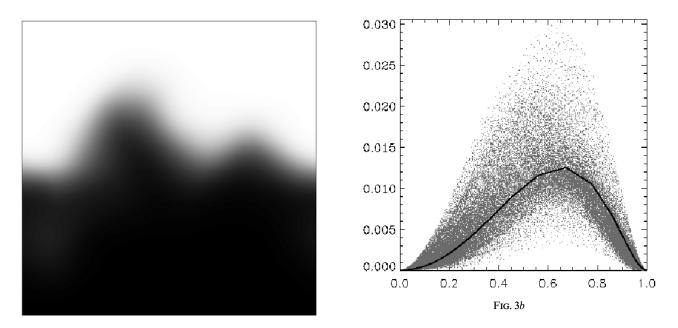


FIG. 3a

FIG. 3.—(a) Snapshot of the scalar field c for $S_{\text{lam}}/u' = 0.95$ and $\Pr = 0.05$. (b) Scalar dissipation rate $(\nabla c)^2$ as a function of c at a fixed time. Superposed is the line corresponding to the laminar solution.

accounting for small-scale turbulence-flame interactions needs to be developed.

All the currently discussed scenarios for deflagrationdetonation transitions (DDT) in the late stage of SN Ia explosions require an earlier transition to distributed or well-stirred burning in order to allow preconditioning of unburned material. Our results indicate that the flamelet structure of thermonuclear flames is more robust than previously anticipated, hence delaying or even preventing the formation of favorable conditions for DDT during the first expansion phase. A more detailed investigation of this question, extending the parameter range to lower $S_{lam}/v(\delta)$, is underway.

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