Numerical simulation of low Mach number reacting flows

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Abstract. The explosion of a Type Ia supernova (SNIa) begins as a turbulent flame deep within a 1.4 solar-mass white dwarf. Initially the burning happens in the flamelet regime where turbulence only serves to wrinkle and fold an essentially laminar burning front. However, as the star expands and the flame moves outwards, it encounters regions of lower density. At $\sim 2 \times 10^7$g cm^{-3}, the flame transitions to a distributed burning regime. Here individual flamelets are disrupted by turbulent eddies, resulting in a fundamental change in the character of the burning. Detonation does not occur immediately because the turbulently broadened flamelets are still too thin. As the density declines further, however, each flamelet thickens and moves faster until only a few structures are contained within the $\sim$ 10 km integral scale of the SN turbulence. It is here that detonation may occur. We present simulations using both a three-dimensional low Mach number model and a one-dimensional linear eddy model to explore the structure of these flames and quantify their scaling behavior. Our results suggest that detonation may be possible at a density near 1.0×10^7 g cm^{-3}.

1. Introduction

It is widely believed that in order to explain the observations of especially the brightest Type Ia supernovae, nuclear burning that remains subsonic at all times (deflagration) is inadequate [1, 2]. There must be, at late times after the star has already expanded significantly, a transition to a more rapid form of burning, i.e., detonation. So far, "delayed detonation" has been introduced into the models as a free parameter, typically an *ad hoc* function of density and turbulent energy [1, 3]. We seek here to understand the physics of the transition and to determine the conditions.

Two previous papers explored the conditions that might lead to a low-density transition to detonation [4] and the nature of turbulent carbon burning resolved in 3D [5]. Here we focus on flames with a fuel of 50% carbon and 50% oxygen at a density of 1×10^7g cm^{-3}, which corresponds to the distributed regime. Through a sequence of simulations, we explore the scaling behavior of flames in this regime and compare the behavior with results using the Linear Eddy Model (LEM;[6]) and with Damköhler scaling [7]. Having verified the 1D LEM, calculations are carried out on still larger scales. We find a transition in the nature of the burning when the size of an eddy that can burn in a turnover time becomes of order the integral scale [8, 9].

Case	(a)	(b)	(c)	(d)	(e)
Domain size L (cm)	150	1200	9600	8.0×10^4	3.27×10^6
Integral length scale l (cm)	15	120	960	7680	4.92×10^5
Turbulent intensity u' (cm/s)	2.47×10^5	4.93×10^5	9.86×10^5	1.97×10^6	7.89×10^6
Scaled turbulent speed s_T^* (cm/s)	1.9×10^4	7.6×10^4	3.04×10^5	1.21×10^6	1.95×10^7
Scaled turbulent width l_T^* (cm)	140	560	2240	8960	3.58×10^4
3D-sim turbulent speed s_T (cm/s)	1.9×10^4	7.7×10^4	3.4×10^5	-	-
3D-sim turbulent width l_T (cm)	140	750	3200	-	-
LEM calculated speed s_T^* (cm/s)	1.5×10^4	6.1×10^4	2.3×10^5	8.2×10^5	1.1×10^7

Table 1. Simulation properties - "scaled" values assume Damköhler scaling ($l^{2/3}$) based on case (a) [5].

2. Methodologies

The three-dimensional simulations are based on the low Mach number model derived from the compressible flow equations using asymptotic analysis to decompose the pressure into dynamic and thermodynamic components. This analytically removes acoustic waves, and therefore the need to resolve them numerically; the equation of state constrains the evolution. The low Mach number equations are discretized using a fractional-step, projection algorithm and coupled to a parallel adaptive mesh framework. For details of the derivation of the method for general equations of state and the numerical method, see [10].

The Linear Eddy Model [6] is a numerical technique that captures many of the aspects of 3D turbulence on a 1D grid. A background isotropic turbulence obeying Kolmogorov statistics is assumed and the action of eddies on a field of abundances and temperature is represented by an instantaneous map (a so called triplet map). Eddy locations are random and size sampling is based on Kolmogorov scaling. The triplet map captures compressive strain and rotational folding effects of eddies and causes no property discontinuities. This approach simulates evolution along a 1D line-of-sight through a 3D flow.

3. Computations and results

3.1. 3D direct numerical simulations

We initialized the simulations (Table 1) with the flat laminar flame in a three-dimensional domain initially filled with homogeneous isotropic turbulence. The flame is oriented so that it propagates downward, although gravitational forces are not included. Periodic boundary conditions were prescribed laterally, a free-slip base, and outflow at the upper boundary. The turbulent velocity field was maintained, following [11], by forcing the momentum equations with a superposition of long wavelength Fourier modes with random amplitudes and phases. The forcing term is scaled by density and so is somewhat reduced in the ash. This approach provides a way to embed the flame in a localized turbulent background, mimicking the much larger inertial range that these flames would experience in a SNIa.

Calculations were carried out for several values of integral scales assuming a constant energy dissipation of $u'^3/l = 10^{15}$ erg g^{-1} s^{-1}. This is on the low end of turbulent intensities expected in an actual supernova [12]. We began with the distributed flame from [5], which has an effective cross-section resolution of 256×256 zones and size 150×150 cm. By demonstrating that we can approximately recover the same turbulent flame speed when the simulation is repeated at a resolution coarsened by a factor of 8 in each direction, we established confidence in simulations with that cell width. Therefore, we can simulate a distributed flame in a 12×12 m domain. This step is then repeated to obtain even larger domains

Fig. 1 shows instantaneous vertical slices of fuel consumption rate (intense burning in red,

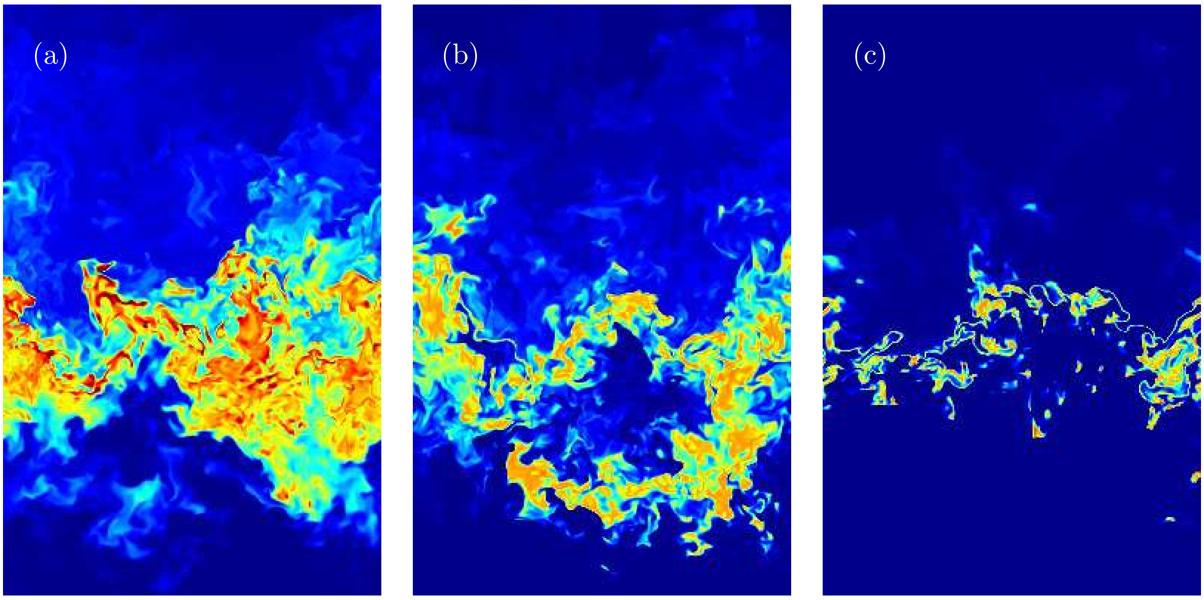

Figure 1. Instantaneous vertical slices of fuel consumption rate (intense burning in red, no burning in blue). The whole domain width is shown but the height is cropped.

no burning in blue). As the flame burns in increasingly larger integral length scales, there is a decrease in the relative size of the flame structures, with burning occurring in distributed pockets. Fig. 2 shows that the flame speed, averaged across the burning volume, is nearly constant after a start up transient. Moreover, taking the $l = 15$ cm case as a base state [5], the steady state speed scales as $l^{2/3}$, the expected scaling for a diffusive flame in which the diffusion coefficient is dominantly due to turbulence ($D \sim u'l$). This scaling must eventually break down due the restriction $s_T \leq u'$.

3.2. 1D results using LEM

Table 1 shows that LEM is able to reproduce well the bulk speeds and widths of the flames calculated in 3D. The speed also obeys Damköhler scaling, but is, over all, a little smaller than the DNS results. Near perfect agreement could have been achieved (but was not) by an adjustment of a parameter in LEM. Heartened by the agreement, we used LEM to explore flame properties on larger length scales than could be done at high resolution in 3D, to 10 km and beyond. Zoning ranged from 0.24 cm for $l = 15$ cm (2048 zones) to 50 cm for $l = 4.5$ km (65536 zones). Until 4.5 km, the $l^{2/3}$ scaling found for smaller integral scales is approximately maintained, but a little below that length scale the flame speed saturates at u'. Above that value, the width and speed are found to scale as $l^{1/3}$, i.e., the turbulent flame speed remains pegged to the the overall turbulent speed on the integral scale. As the integral speed approaches this value, the flame front became complex (Fig 2) and the burn rate irregular. Variations in integrated burning rate of about a factor of three were observed (the values in Table 1 are averages), and the carbon mass fraction in the burning region was about three times less than that in the fuel, corresponding to an overall reduction in burning time scale of a factor of 9.

4. Conclusions

Figure 3 [9] summarizes our conclusions and shows where and how detonation might happen in a SNIa. The Karlovitz number is defined as $\mathrm{Ka} = (l_L/l_G)^{1/2}$, where l_L is the laminar flame thickness (where one exists), and l_G is the Gibson scale. For $\mathrm{Ka} < 1$, one has laminar flames,

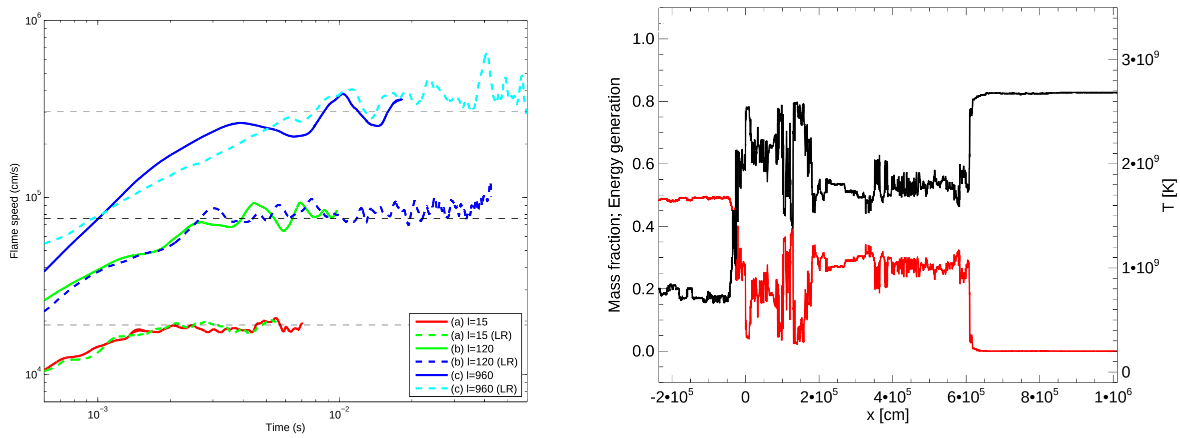

Figure 2. *Left:* Turbulent flame speeds from three-dimensional simulations. Solid lines denote high resolution simulations (256 zones across), dashed lines denote low resolution (LR) simulations (32 zones across). Colors denote same cell width. Dashed lines are turbulent flame speeds predicted by Damköhler scaling. *Right:* A calculation using LEM of a single flame for an integral scale of 4.92 km at a density 1×10^7 g cm^{-3}. The turbulent speed on that scale is 78.9 km s^{-1} and the average flame speed and width are also close to these values. Many complex and folded structures are seen, but occasionally surprisingly homogeneous, isothermal regions appear. Red is carbon mass fraction and black is the temperature.

folded and deformed by turbulence, but each still well defined. No detonation is possible in this regime. The overall burning moves at approximately u^*, the characteristic speed of turbulence on the integral scale of the supernova, L^*, and the individual flamelets serve only to "digest" the entrained fuel. The number of such flames contained within the integral scale is approximately $n \approx u^*/s_L$, with s_L the laminar flame speed, and so can be very large. Above Ka $= 10$ (shown on Fig. 3), turbulence tears individual flamelets and dominates the heat transport. This is the region delimited and studied here in our 3D simulations. For typical turbulence parameters, $L^* = 10$ km and $u^* = 100$ km s^{-1}, we find that the transition to "distributed burning" happens at about 2×10^7 g cm^{-3}.

For lower densities or higher turbulent speeds, Ka > 10, i.e., as the supernova expands further, one still has a large collection of flamelets within L, but each flamelet becomes broadened and accelerated by the turbulence. At a given density and turbulent energy dissipation, $\varepsilon = u^{*3}/L^* \sim 10^{15} - 10^{18}$ erg g^{-1} s^{-1} for $u^* = 100$ to 1000 km s^{-1}, there is a characteristic length scale, $\lambda = (\tau_{nuc}^3 \varepsilon)^{1/2}$ [8, 4]. This is the size of an eddy that will burn in a turnover time (a macroscopic analogue, for turbulent flames, of the Gibson length). The characteristic nuclear time, τ_{nuc}, is evaluated in our studies and is $\tau_{nuc} = l_T/s_T$ in Table 1. There is only one physical integral scale in the supernova, $L^* \sim 10$ km, but we explored the scaling properties of the turbulent flame speed and width by varying a fictitious integral scale, l, subject to the constraint $\varepsilon =$ constant (Table 1), confirming the expected Damköhler scaling, $s_T \propto l^{2/3}$ and $l_T \propto l^{2/3}$ so long as $l < \lambda$. The ratio $(L^*/\lambda)^{2/3} = L^*/(u^* \tau_{nuc})$ is also known as the Damköhler Number.

So long as Da $\gg 1$, i.e., $\lambda \ll L^*$, there are still many turbulently broadened flamelets, each of width $\sim \lambda$, contained within the integral scale. Stochastic variations in the speeds of individual flamelets will tend to cancel out because $\sqrt{n}$ is large. However, as Da approaches unity, the flamelets become fewer and broader, and move faster. Eventually, at Da $= 1$, there is, on the average, only one flame with width L^* and speed u^*. It is here that our studies with LEM show that the overall flame speed exhibits large fluctuations. The flame structure is very complex with transient large regions of mixed fuel and ash. "Microexplosions" occur as these pockets burn nearly coherently.

Increasing the turbulence still further, or decreasing the density (hence increasing τ_{nuc} and λ and decreasing Da below 1), does not help. One would then get a single turbulently broadened flame with width $\lambda > L^*$, and speed $< u^*$, similar to the ones studied here in 3D. Thus if detonation is to happen, it happens for Da $\approx$ 1 - 10. Our studies with LEM [9] show that the maximum boost from the irregular burning of the flame in this regime corresponds to a reduction in burning time scale of at most a factor of 9. Thus to get supersonic burning, one must also have turbulent speeds no slower than about 10% sonic [12]. Finally the region that burns faster than sound must large enough to initiate a self-sustaining detonation [4]. Our calculations show that all these conditions may be simultaneously satisfied at 10^7 g cm^{-3}, though not by a large margin.

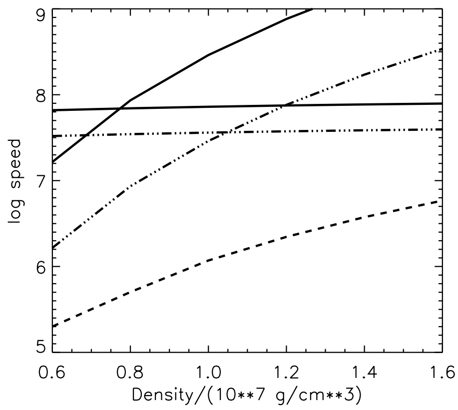

Figure 3. Regions of distributed burning. The y-axis is the log of the turbulent speed on an integral scale, L^*, assumed to be 10 km, and the x-axis is density. The lowest dashed line is Ka = 10. Below this line, one is in the laminar flamelet regime. The solid and dot-dashed slowly rising lines are Da = 1 and 2 respectively. The solid and dot-dashed nearly horizontal lines are sound speed divided by 5 (lower line) and 10. See [9] and text.

Acknowledgments
A. Aspden was supported by a Seaborg Fellowship at LBNL under DOE contract DE-AC02-05CH11231. J. Bell was supported by the SciDAC Program under contract No. DE-AC02-05CH11231. This research used resources of the National Center for Computational Sciences at Oak Ridge National Laboratory, which is supported by the Office of Science of the DOE (DE-AC05-00OR22725). Additional computing resources were provided on the ATLAS Linux Cluster at LLNL as part of a Grand Challenge Project. Work at UCSC was supported by SciDAC (DE-FC02-06ER41438). Sandia Laboratory is operated by the Sandia Corporation, a Lockheed Martin Company, for the DOE under contract DE-AC04-94AL85000.

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