Astrophysical Combustion: From a Laboratory Flame to a Thermonuclear Supernova

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1 Introduction

Exothermic processes associated with nuclear fusion and fission reactions are of fundamental importance in astrophysics. From the first moments of the Big Bang, nuclear reactions have been the primary driver shaping the observable baryonic Universe. Such processes predominantly have two manifestations: slow, more gentle hydrostatic "simmering" found in stable stars, such as the Sun, during most of their evolution and violent explosive burning that occurs in astrophysical transients.

Despite seeming vast differences, burning in astrophysical plasmas and chemical systems on Earth bears many similarities. This particularly concerns situations with explosive burning, which are the main focus in this paper. In both cases, flow dynamics can be described using continuum Navier-Stokes equations with the energy source terms and microphysical transport processes [1]. While astrophysical plasmas are often magnetized, in many systems field strengths are well below equipartition and, thus, magnetic effects can be neglected. Furthermore, explosive thermonuclear burning often occurs in the form of flames and detonations, with the overall structure and dynamics similar to that of their terrestrial counterparts.

Thermonuclear reactions take place at conditions, which are very different from those present in chemical combustion. For instance, in the case of explosive ¹²C burning found in thermonuclear (type Ia) supernovae, product temperatures exceed 10⁹ K and can be as high as 10¹⁰ K. Furthermore, fusion reactions typically have much stronger temperature dependence, thus, representing some of the most nonlinear processes found in the Universe [1]. Figure 1a shows the activation energy, T_a , of some of the key individual ¹²C-burning reactions, as well as the effective T_a in laminar thermonuclear flames for a range of densities and fuel compositions. It can be seen that T_a is remarkably large being well in excess of 10¹⁰ K. At the same time, seemingly paradoxically, the corresponding characteristic Zel'dovich numbers, Ze, in ¹²C flames (Fig. 1b) are very similar to those found in chemical flames, becoming somewhat larger only at low densities ~10⁶ g/cm³.

The largest differences between chemical and astrophysical combustion lie in terms of the equation of state and the microphysical transport processes. In particular, in the core of a white dwarf or on the surface of a neutron star, plasma becomes degenerate, which dramatically changes its equation of state with pressure becoming virtually independent of temperature. As a result, thermonuclear flames have a very low degree of expansion with the density jump across the flame typically <2. In contrast, chemical flames under normal, atmospheric conditions have much larger density ratios ~6-10. At the same time, at high fuel pressures and temperatures the density ratio across the flame can decrease significantly. For instance, for a realistic jet fuel (n-dodecane) adiabatically compressed to the pressure of 30 bar and temperature of ~800 K, which is representative of the realistic jet-engine operating conditions, the density ratio across a premixed flame is only ~3.6.

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Figure 1. Activation temperature, T_a , (a) and the corresponding Zel'dovich number, Ze, (b) calculated along the laminar flame profiles for a range of densities given in the legend in panel (a) [7]. Solid color lines correspond to the upstream carbon mass fraction $X_{C,0} = 0.5$, dashed color lines correspond to $X_{C,0} = 0.2$. Dashed red line represents pulsatingly unstable flame. In panel (a), black solid lines show the analytically calculated profiles of T_a for several fundamental reactions based on the unscreened reaction rates by Caughlan & Fowler [2]. All color curves were calculated using a thermonuclear α -network. They are shown only for temperatures between 8×10^8 K, at which reactions in the flame become non-negligible, and the ¹²C-burning temperature, T_C , in the flame profile, i.e., temperature corresponding to $X_C = 0.05X_{C,0}$.

Degenerate (and often relativistic) electron gas in the plasma also alters transport properties, greatly enhancing thermal conduction compared to species diffusion resulting in the incredibly large characteristic Lewis numbers $Le \sim 10^4 - 10^7$ and Prandtl numbers $Pr \rightarrow 0$.



Figure 2. Comparison of the structure of a chemical (solid lines) and thermonuclear flame (dashed lines). Chemical flame structure is calculated for a stoichiometric jet-fuel (n-dodecane) – air mixture under atmospheric conditions using a reduced 24-species reaction network [8]. Thermonuclear flame is calculated for a 50/50 12 C/ 16 O fuel at the density $\rho = 5 \times 10^7$ g/cm³ using a 13-isotope α -network [9]. The *x*-coordinate is normalized by the laminar flame thermal width for a chemical flame and by the width of the 12 C-burning zone for a thermonuclear flame. Energy release rate is normalized by its peak value, density and temperature are normalized as ($\varphi - \varphi^{min}$)/($\varphi^{max} - \varphi^{min}$), where φ represents either ρ or *T*.

Despite these large differences in the microphysical properties, resulting chemical and thermonuclear flames have a very similar structure. This is illustrated in Fig. 2, which shows the normalized profiles of density, temperature, and energy release rate for a chemical (jet-fuel-air) and thermonuclear (degenerate plasma with 50/50 12 C/ 16 O composition) flames. First, at the conditions selected here (atmospheric conditions for a chemical flame, and density $\rho = 5 \times 10^7$ g/cm³ for a thermonuclear

flame), thermal width of a chemical flame (0.4 mm) is very close to the width of the ¹²C-burning zone in a thermonuclear flame (0.5 mm). Furthermore, remarkably, normalized profiles of energy release rate are virtually identical in both cases, as can be seen in Fig. 2. The laminar flame speeds, however, differ by almost 4 orders of magnitude (\sim 34 cm/s for jet-fuel–air vs. \sim 1 km/s for degenerate plasma).

Dynamically, laminar thermonuclear flames exhibit instabilities similar to those of their chemical counterparts, e.g., thermodiffusive (pulsating) instability associated with large Le [2], hydrodynamic (Landau-Darrieus) instability [3], and body-force (Rayleigh-Taylor) instability [4]. They also have similar response to stretch, with the characteristic Markstein numbers of order unity [5]. Structure of thermonuclear detonations is well described using the classical Zel'dovich-von-Neumann-Döring theory, and they exhibit similar types of the multidimensional cellular instability found on Earth [5].

2 Chemical and Thermonuclear Combustion: Possible Synergy?

Understanding of the large-scale dynamics of astrophysical combustion systems, e.g., type Ia supernovae, requires solution of numerous challenges similar to those faced by the chemical combustion community:

- autoignition in a turbulent flow,
- properties of turbulent flames, in particular the ability to predict turbulent flame speeds,
- mechanisms of detonation formation and the nature of deflagration-to-detonation transition,
- properties of detonations, i.e., their stability, response to curvature, propagation through strongly inhomogeneous mixtures, etc.

Furthermore, similarly to the terrestrial combustion systems, theoretical studies of the interplay between small-scale properties of thermonuclear flames and detonations and the overall dynamics of their host systems critically require numerical modeling. However, in astrophysical systems, one encounters two key complications. First, the dynamical range of scales, which must be considered, is typically vastly larger than on Earth with the size of the combustion system, e.g., a white dwarf star, being many orders of magnitude larger than the characteristic combustion scale, e.g., a flame width. Second, unlike on Earth, results of numerical modeling cannot be directly tested with a suitable experiment. Instead, their validity can be assessed only through comparison with the observational signatures of the object in question. Since the initial state of the system is typically completely unknown, interpreting such observational data is often difficult and such interpretation inherently relies on the assumed physical model of the combustion process.

In light of strong similarities, as well as important differences, between chemical and astrophysical combustion in terms of the underlying physical model, it is well warranted then to ask the following two questions.

1) Can theoretical, numerical, and experimental advances in terrestrial combustion help address open problems in astrophysical combustion mentioned above?

2) Conversely, can astrophysical systems provide a unique and complementary (in terms of extreme spatial and temporal scales, physical conditions, etc.) test bed for our understanding of the dynamics of flames and detonations?

An example of the synergy between chemical and astrophysical combustion is shown in Fig. 3. One of the key outstanding open challenges in the theory of thermonuclear supernovae is the question of the nature of a spontaneous deflagration-to-detonation transition (sDDT) in unconfined systems. In our previous work [10], we identified a new mechanism of sDDT, which occurs in fast turbulent flames propagating with speeds faster than the speed of a Chapman-Jouguet (CJ) deflagration. Criteria for the minimal turbulent integral scale, l, and velocity, U_l , required for sDDT to occur are [9]

$$\frac{l}{\delta_L} = \left(\frac{A_{\delta}}{B_L}\right) \frac{c_s}{\alpha I_M S_L}; \quad \frac{U_l}{S_L} = \alpha I_M \left(\frac{l}{\delta_L}\right)^{1/3}; \quad A_{\delta} \approx 2; \quad B_L \approx 10; \quad I_M \approx 0.65 - 0.85$$
(1)



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Figure 3. *Left:* traditional combustion regime diagram for stoichiometric, atmospheric H₂-air flames, showing unstable regimes (shaded gray region), in which unconfined turbulent flames spontaneously undergo the deflagration-to-detonation transition (DDT). Minimum *l* and U_l in the shaded gray region are calculated using eq. (1). Red diamonds mark direct numerical simulations (DNS), in which spontaneous DDT was observed [10], while black circles and green stars represent calculations, in which turbulent flames were found to be either quasi-stable or pulsatingly unstable periodically producing pressure waves [11, 12, 13]. *Right:* Critical system sizes for spontaneous DDT in thermonuclear flames based on eq. (1) normalized by the width of a ¹²C-burning zone. Dashed and solid lines correspond to pure ¹²C and 50/50 ¹²C/¹⁶O fuel, respectively. Shaded gray region shows the system size, which can be modeled using modern computational resources. Shaded red region shows the predicted range of densities, above which spontaneous DDT can be observed in DNS that are computationally feasible today.

Here, S_L and δ_L are the laminar flame speed and width, c_s is the sound speed, α is the density ratio across the flame, I_M is the stretch factor (related to the Markstein number), and A_s and B_L are constants representing, respectively, the ratios of the minimal flame separation in the flame brush to δ_L and of the overall turbulent flame width to l.

A systematic survey of a large range of turbulent conditions for chemical flames using both singlestep, Arrhenius-type reaction models as well as the detailed chemical kinetics representative of H_2 combustion showed the validity of this model. In particular, the range of unstable regimes for stoichiometric H_2 -air mixtures based on eq. (1) is shown in the left panel of Fig. 3 as the shaded gray region. It can be seen that it accurately captures both the minimum system size and turbulent intensity, at which sDDT was observed in DNS calculations (cf. red diamonds vs. black circles and green stars).

This model, which was validated for chemical flames, was subsequently used to predict the range of unstable regimes for thermonuclear flames. In particular, we used it to determine the fuel composition and minimal system size, L^{min}_{CJ} , at which sDDT can occur in a direct numerical simulation (DNS) that is feasible today using modern computational resources. The range of system sizes accessible to modern state-of-the-art DNS is shown as the shaded gray region in the right panel of Fig. 3. It can be seen that for 50/50 12 C/ 16 O mixtures, the critical system size remains above this range practically for all densities of interest as high as 10^9 g/cm³. At the same time, for a pure 12 C fuel, sDDT can be captured in DNS at densities above ~1.5 - 3×10^8 g/cm³. DNS of turbulent thermonuclear flames that we carried out at a slightly higher density, namely $\rho = 4 \times 10^8$ g/cm³, indeed showed the formation of a super-CJ flame, which produced a strong shock wave. Detailed discussion of these results is presented in a separate paper [9].

This shows that understanding developed through studies of chemical reacting flows can provide not only qualitative, but also quantitative guidance, which is directly applicable to thermonuclear combustion in degenerate plasmas.

3 Special Session at ICDERS 2015: Starting the Dialog

The goal of the special session on astrophysical combustion at the ICDERS 2015 meeting is to promote the dialog between the astrophysical and chemical combustion communities with the aim of answering the two questions posed above. In particular, it is intended to:

- facilitate the exchange of theoretical advances and numerical tools between the communities,
- identify areas of common interest, in which cross-disciplinary collaboration can lead to the advancement of the state-of-the-art in both communities,
- encourage development of experimental settings, which can help answering astrophysically relevant questions.

This talk will give an overview of the similarities and differences in terms of the physical model between chemical and astrophysical combustion, as well as of the open challenges facing both communities, as discussed above. The goal of this talk is to provide an introduction for the subsequent presentations in this special session.

References

[1] Timmes F.X., Woosley, S.E. (1992), Astrophys. J., 396, 649.

[2] Poludnenko A.Y., Gamezo, V.N., Oran, E.S. (2015), in preparation.

- [3] Bell J.B., Day M.S., Rendleman C.A., Woosley S.A., Zingale M. (2004), Astrophys. J., 606, 1029.
- [4] Bell J.B., Day M.S., Rendleman C.A., Woosley S.A., Zingale M. (2004), Astrophys. J., 608, 883.

[5] Dursi L.J. et al. (2003), Astrophys. J., 595, 955.

- [6] Gamezo V.N., Wheeler J.C., Khokhlov A.M., Oran E.S. (1999), Astrophys. J., 512, 827.
- [7] Caughlan G.R., Fowler W.A. (1988), At. Data Nucl. Data Tables, 40, 283.
- [8] Gao Y. et al. (2015), Combust. Flame, in press.
- [9] Poludnenko A.Y., Taylor B.D. (2015) submitted.
- [10] Poludnenko A.Y., Gardiner T.A., Oran E.S. (2011), Phys. Rev. Lett., 107, 054501.
- [11] Poludnenko A.Y., Oran E.S. (2010), Combust. Flame, 157, 995.
- [12] Poludnenko A.Y., Oran E.S. (2011), Combust. Flame, 158, 301.
- [13] Poludnenko A.Y. (2015), Phys. Fluids, 27, 014106.