A one-dimensional model for accelerating deflagrations and their transition to detonations

Willstrong Rakotoarison, Hongxia Yang, Matei I. Radulescu
University of Ottawa, Department of Mechanical Engineering
Ottawa, Ontario, Canada

1 Introduction

In the study of accelerating deflagrations and their transition to detonation, the main mechanisms leading to an overall increase of the burning rate are multi-dimensional. They include flame stretching and folding mostly due to preferential convection in tubes, hydrodynamic and thermal-diffusive instabilities, or interaction with turbulence, shocks or boundary layers, as well as their interactions [1–3]. Despite the complexity of these events, it is observed in shock tube experiments and numerical simulations, that flames reach a quasi-steady propagation regime known as the *choking regime* [4], during which it forms, strenghtens and drives pressure waves and shocks ahead of itself [3, 5, 6]. Those eventually become strong enough to, later on, allow thermal initiation of a detonation by shock pre-heating or by the formation of hot-spots at shock reflection locations, in the presence of solid walls [7].

This general view of the sequence of events suggests that a simpler, one-dimensional problem can be formulated to study the overall flow field involved in flame acceleration problems, in which the deflagration transition to detonation is controlled only by simple gasdynamical processes. The approach chosen in this paper was to artificially control the flame burning rate, in order to trigger a response of the flow, typically the formation of compression waves in the fresh gases when the burning rate increases. Here, altering the flame burning rate is done by modulating the pre-exponential factor of the one-step, irreversible, Arrhenius type law used to describe the depletion rate of reactants. Doing so permits to generate flow-fields relevant in accelerating flame problems, and better investigate the nature of the interaction between the flame and their compressible features. Special attention will be addressed to the case of high speed deflagrations, propagating near the Chapman-Jouguet (CJ) deflagration conditions. Those are associated to choked flames in shock tube experiments [8] and are, by definition, deflagrations propagating with a sonic downstream flow, at the theoretical highest burning velocity a subsonic flame could propagate at.

2 Governing equations and numerical setup

One-dimensional deflagrations were modeled using the reactive Navier-Stokes equations, with single-step, irreversible, first-order chemical reaction rate. They were non-dimensionalized in a manner identi-

Correspondence to: wrako027@uottawa.ca

cal to the work of Sharpe [9]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) = \mathrm{Pr}\frac{4}{3}\frac{\partial^2 u}{\partial x^2} \tag{2}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}(Eu + pu) = \frac{\gamma}{\gamma - 1}\frac{\partial^2 T}{\partial x^2} + \mathrm{Pr}\frac{4}{3}\frac{\partial}{\partial x}\left(u\frac{\partial u}{\partial x}\right) + Q\omega \tag{3}$$

$$\frac{\partial}{\partial t}(\rho Y) + \frac{\partial}{\partial x}(\rho u Y) = \frac{1}{\mathrm{Le}}\frac{\partial^2 Y}{\partial x^2} - \omega \tag{4}$$

$$\omega = \Lambda \rho Y \exp\left(\frac{-\theta}{T}\right) \times H(T - T_i) \tag{5}$$

where $p = \rho T$, $E = \rho T/(\gamma - 1) + \rho u^2/2$, H is the Heaviside function and T_i an ignition temperature below which no chemical reactions occur and typically set slightly above the unburned, undisturbed gases temperature. The following reference scales were used:

$$\rho = \frac{\overline{\rho}}{\overline{\rho}_u} \quad , \quad u = \frac{\overline{u}}{\overline{S_f}} \quad , \quad x = \frac{\overline{u}_u}{\overline{\alpha}_u}\,\overline{x} \quad , \quad T = \frac{\overline{R_g}}{\overline{S_f}^2}\,\overline{T} \quad , \quad \theta = \frac{\overline{Ea}}{\overline{S_f}^2} \quad , \quad Q = \frac{\overline{Q}}{\overline{S_f}^2} \tag{6}$$

Variables ρ, u, T, Y, p, $M_f = u_u/c_u$ and $c = \sqrt{\gamma p/\rho}$ are respectively the gas density, flow velocity, temperature, mass fraction of fresh gases, pressure, flame burning Mach number and speed of sound. Variables denoted with an over bar relate to dimensional quantities, those with index (u) to their value taken in the unburned and undisturbed gases.

The relevant dimensional gas properties are $\overline{S_f}$, $\overline{\nu}_u$, $\overline{\alpha}_u$, $\overline{D}_u$, $\overline{R_g}$, $\overline{Q}$, $\overline{Ea}$ and $\overline{k}$, respectively the flame burning velocity, gas kinematic viscosity, thermal and molecular diffusivity coefficients, the specific perfect gas constant, heat of reaction, activation energy and reaction rate pre-exponential factor, also referred to as the *burning rate eigenvalue* [10]. They are used to define the dimensionless heat of reaction Q, activation temperature θ and burning rate eigenvalue Λ, as well as the other commonly used and later useful non-dimensional energies $\widetilde{Q} = \overline{Q}/(\overline{R_g}\,\overline{T_u})$ and $\widetilde{Ea} = \overline{Ea}/(\overline{R_g}\,\overline{T_u})$. Finally, the non-dimensional parameters $\mathrm{Pr} = \overline{\nu}_u/\overline{\alpha}_u$ and $\mathrm{Le} = \overline{\alpha}_u/\overline{D}_u$ are the Prandtl and Lewis numbers, respectively equal 3/4 and 1.

In the present study, the value of Λ is varied over time to cause the flame burning rate to change accordingly. The numerical simulations aimed to model flame acceleration are thus performed as follow. The profiles of a steady flame propagating at a given burning Mach number M_{f0} are found using the method described in the previous work [11], together with the matching burning rate eigenvalue Λ_0. The profiles were imported as initial conditions in a hydrodynamical solver. The flame was left to propagate steadily for some time, typically over 10 times the characteristic particle flame crossing time, to ensure it keeps its original structure and eventual numerical disturbances fade far from the reaction zone. The value of Λ was then increased linearly over time from $t = t_0$, i.e.:

$$\Lambda(t) = \Lambda_0 + \left(\frac{d\Lambda}{dt}\right)_0 (t - t_0) \tag{7}$$

where Λ_0 corresponds to the initial burning rate eigenvalue calculated for the steady flame set as initial conditions, and $\left(\frac{d\Lambda}{dt}\right)_0$ its increase rate, typically equal to a fraction of Λ_0. This causes the flame to accelerate and generate disturbances upstream and downstream of the reaction zone, until it eventually transits to a detonation.

The simulations were performed on a numerical solver developed by Falle [12, 13]. Convective terms were solved using a second order accurate Godunov scheme, and diffusion terms were solved explicitly in time, using second order central differences in space. Zero-gradients conditions were set at the boundaries of the domain to approximate an open tube. The domain was discretized to provide 1/4 of a cell per unit length (1 cell covers 4 unit lengths), and adaptive mesh refinement was used [14] to provide details in high gradients regions, typically the reaction zones and shocks, allowing for a maximum resolution of 48 cells per unit length, i.e. about 100 cells per thickness of the non-disturbed flame.

3 Results and discussion

The parameters γ, $\widetilde{Ea}$ and $\widetilde{Q}$ were chosen to be 1.4, 50 and 50. The initial flame was set to propagate at a Mach number $M_{f0} = 0.11$. This value is close to the CJ deflagration Mach number for the chosen set of parameters, equal to $M_{CJ} = 0.119$. The associated burning rate eigenvalue was thus found to be $\Lambda_0 = 2.65 \times 10^3$.

The flame was set to accelerate from time $t_0 = 40$, by increasing the value of Λ following the relation (7), where $\left(\frac{d\Lambda}{dt}\right)_0 = 5.90$, that corresponds to 0.22% Λ_0. The resulting flow can be visualized in the space-time diagrams plotted in Figures 1, showing density in gray scale. Plot (a) shows the overall flame acceleration process. At the very early times, the flame is steady and thus does not drive compression waves in the fresh gases. When the flame starts to accelerate, it generates and amplifies a shock ahead of it, that can be seen clearly in Figure 1(a). Its strength is annotated on the same figure at different space-time coordinates. At later times, the density jump across the shock propagating at a Mach number of about 2.2 is obvious, as seen on Figure 1(b), behind which the density increases monotonously until it reaches a maximum just ahead of the reaction zone. This density gradient can be seen on the few first density profiles plotted in Figure 2. Around time 2730, the deflagration transits to a detonation due to an explosion occurring just ahead of the reaction zone. The detonation then travels in the shocked region until it catches up the shock wave around time 2790.

This sequence of events is typical of what was observed for other values of $\left(\frac{d\Lambda}{dt}\right)_0$, and differs only in the timing at which the shock forms and transition to detonation occurs. For high values of $\left(\frac{d\Lambda}{dt}\right)_0$, i.e. for highly accelerating flames, transition to detonation happens earlier than for low values. This result was anticipated, owing to the shock being stronger at earlier times, thus providing the conditions required for thermal explosion more rapidly. Interestingly, this rapid shock formation occurs when the deflagration reaches a burning rate equal to the CJ conditions, here around time 500. This can be seen on Figure 3, where are plotted as a function of time the flame Mach number in black, and the CJ deflagration Mach number in red, both calculated taking as fresh gases conditions the state just ahead of the flame.

Later on and as seen in Figure 3 between times 500 and 1500, the flame remains in the CJ conditions despite the fact that its burning rate continuously increases. This is caused by the coupling between the shock and the flame: as the former gets continuously stronger and its downstream state hotter, the flame propagating conditions are changed such that larger CJ deflagration burning velocities are allowed, thus permitting the flame to keep accelerating and strengthen the shock. As seen on Figure 3, this feedback mechanism goes on until time 1500, where the flame burning rate starts to oscillate around the CJ deflagration conditions. The amplitude of the oscillations increases until the deflagration transits to a detonation. This novel flame instability observed just prior to transition appears to be a gasdynamic pulsating instability characteristic of gasdynamic coupling, usually present in detonation waves. Such high frequency instabilities have been observed near detonation transition in accelerating flames in narrow tubes and re-initiation start of the galloping detonations [15]. Although numerical artifacts cannot be completely ruled out, our simulations reproducibly predicted such oscillations for all the acceleration ramps investigated.

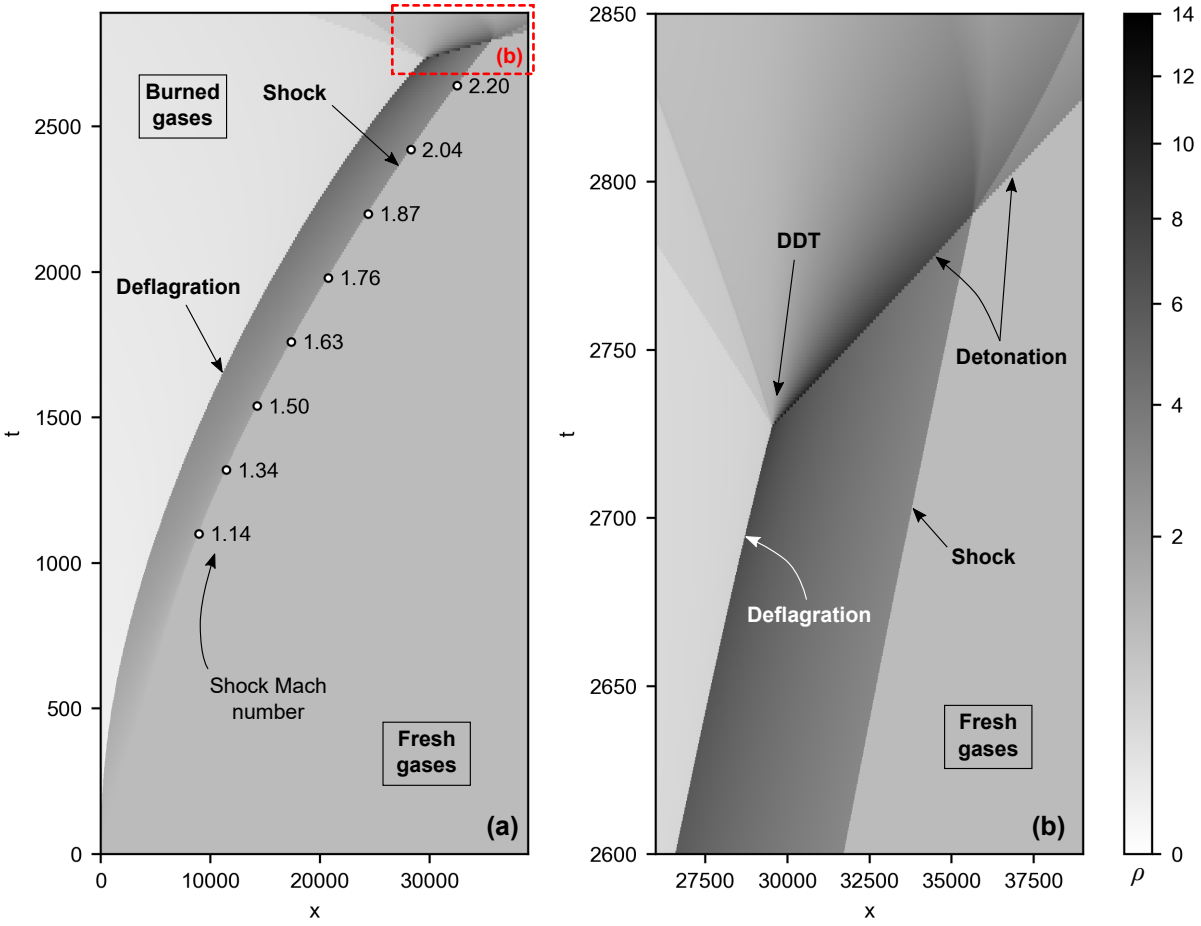

Figure 1: Space-time diagram plotted for density of the flame acceleration process. (a) shows the overall evolution of the flame and the shock, which strength is annotated along its trajectory. (b) shows the late stages of the flame acceleration process, where transition to detonation occurs.

These simulations were repeated starting with flames propagating at significantly lower values of the initial burning rate, far from the CJ conditions. In this case, the flame did not contribute to form shocks strong enough to allow the gases to ignite over a reasonably short time. This is consistent with the numerical work of Fecteau [16], in which the evolution of two-dimensional flames and their eventual transition to detonation was investigated. The burning rate of the initial flame was adjusted using the thickened flame model, and evolution to unsteadiness was favored by an initial deformation of the planar flame front. Under these conditions, the perturbation grows, thus increasing the flame surface area, providing the main cause of the global increase of the burning rate. Differences in the following events were found when the burning rate of the planar flame was changed. At low values, the flame eventually settles to propagate steadily. However at high values of the planar flame burning rate, a shock eventually forms in the fresh gases. When the planar flame burning rate was set to be close to the CJ conditions, transition to detonation occurred rapidly. This sequence of events is also consistent with experimental observations, where the increase of the burning rate is mostly provided by the deformation of the flame front, due to the presence of solid walls, to the interaction with the turbulence, or interaction with shocks and boundary layers. At the later stages of flame acceleration, strong shocks form rapidly when the flame eventually reaches conditions close to CJ deflagrations, i.e. the choking regime, supporting the initiation of detonations [17–21].

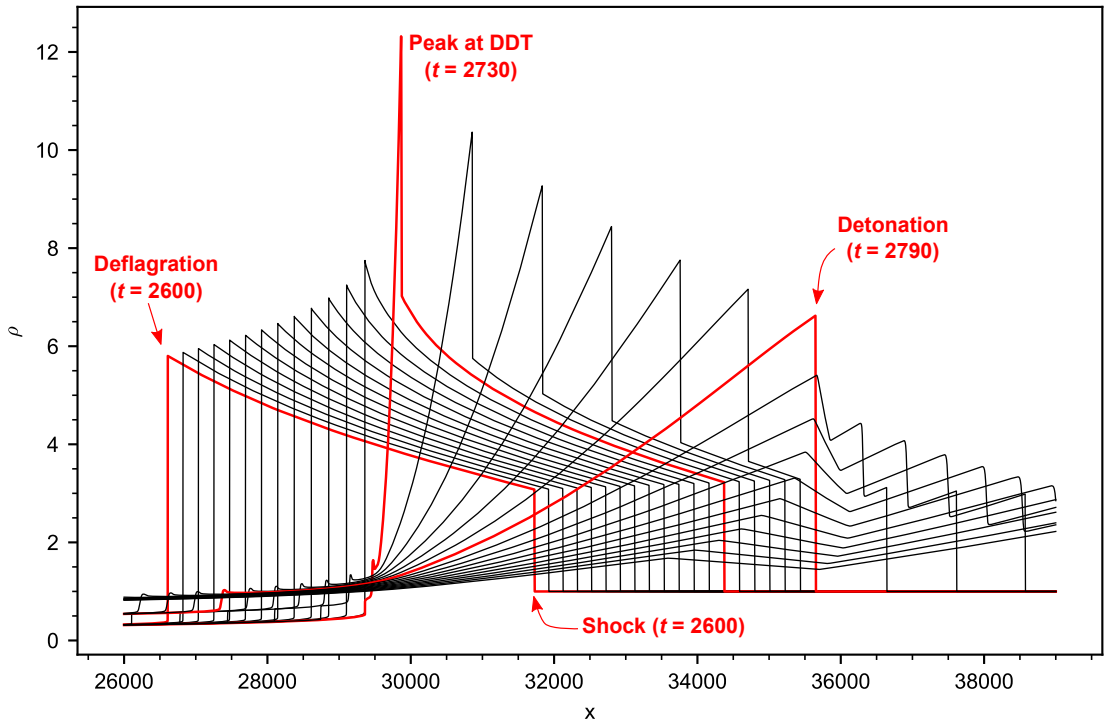

Figure 2: Series of density profiles plotted around the time of transition to detonation (see Figure 1(b)). Time interval between each plot is 10.

The similarities of these results with the one-dimensional evolution of accelerating flames presented in this section suggests that a global description of DDT can be considered. Mostly, CJ deflagrations appear to be important, as they constitute a propagation regime that promotes the formation and growth of shocks strong enough to allow the onset of detonations. It can be seen in Figure 3 that a coupling exists for some time between the shock and the flame. The fact that the flame remains in the CJ conditions while its burning rate is continuously increased, opens the path to models meant to describe in a simple way the resulting flow field. For example, in a manner similar to the two-discontinuities models describing the pseudo-steady flow field involving a shock followed by a CJ deflagration [8, 22], a simple model describing the evolution of an accelerating shock-flame complex can be developed, in which the flame, which burning rate grows but remains in the CJ conditions, causes the strengthening of its precursor shock accordingly. Such a model is currently left as a work in progress.

4 Concluding remarks

The relative simplicity of the simulations presented here made it easy to implement and generate results. The method described in the previous section to model accelerating flames was found to reproduce well the coupling that exists between the flame and the flow field, from the shock formation to the initiation of the detonation. This makes it a convenient tool to reproduce and better understand the overall conditions required for deflagrations to transit to detonations.

A very interesting result here is the role of the shock heating, allowing the deflagration to remain choked over some time, before the fresh gases located just ahead of it are thermally ignited to form a detonation. In this case, the coupling between the deflagration and the shock is such that, the latter's strength increases rapidly under the influence of the following CJ deflagration. With it, the deflagration remains

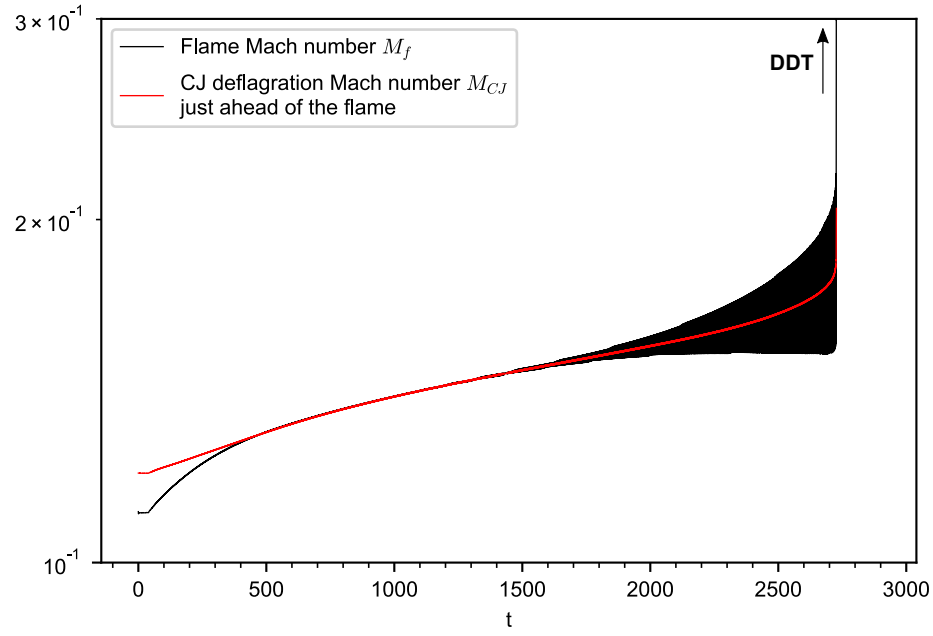

Figure 3: Evolution of the flame Mach number and the expected CJ deflagration Mach number over time.

in the CJ conditions even if its burning rate increases, owing to the continuously changing conditions in the shocked state. This result was expected as deflagrations propagating near the CJ conditions are prone to generate compression waves rapidly in the fresh gases. While the propensity of CJ deflagrations to generate pressure waves is relatively accepted [23–25], the present results show that the deflagration does so in order to remain a CJ deflagration in relation to newly compressed gas just ahead of itself. This self-organization of CJ deflagrations into stronger CJ deflagrations is the first main finding of the present work. The second finding is the onset of detonation being associated with a pulsating instability, akin to the gasdynamic coupling in detonation waves where reaction zones and flames are in phase with each other and yield very rapid amplification [26]. This instability may generate local hot-spots beyond what the lead shock is capable of. Further work should focus on this unique feature of accelerating flames.

References

[1] G. Ciccarelli and S. Dorofeev, "Flame acceleration and transition to detonation in ducts," *Progress in Energy and Combustion Science*, vol. 34, no. 4, pp. 499–550, Aug. 2008.

[2] G. Thomas, R. Bambrey, and C. Brown, "Experimental observations of flame acceleration and transition to detonation following shock-flame interaction," *Combustion Theory and Modelling*, vol. 5, no. 4, pp. 573–594, Dec. 2001.

[3] H. Yang and M. I. Radulescu, "Enhanced DDT mechanism from shock-flame interactions in thin channels," *Proceedings of the Combustion Institute*, vol. 38, no. 3, pp. 3481–3495, Jan. 2021.

[4] J. Lee, R. Knystautas, and C. Chan, "Turbulent flame propagation in obstacle-filled tubes," *Symposium (International) on Combustion*, vol. 20, no. 1, pp. 1663–1672, Jan. 1985.

[5] D. M. Valiev, V. Bychkov, V. Akkerman, and L.-E. Eriksson, "Different stages of flame acceleration from slow burning to Chapman-Jouguet deflagration," *Physical Review E*, vol. 80, no. 3, p. 036317, Sep. 2009.

[6] D. M. Valiev, V. Bychkov, V. Akkerman, L.-E. Eriksson, and C. K. Law, "Quasi-steady stages in the process of premixed flame acceleration in narrow channels," *Physics of Fluids*, vol. 25, no. 9, p. 096101, Sep. 2013.

[7] P. A. Urtiew and A. K. Oppenheim, "Experimental Observations of the Transition to Detonation in an Explosive Gas," *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 295, no. 1440, pp. 13–28, Nov. 1966.

[8] R. S. Chue, J. F. Clarke, and J. Lee, "Chapman-Jouguet Deflagrations," *Proceedings of the Royal Society London. Series A: Mathematical, Physical and Engineering Sciences*, vol. 441, no. 1913, pp. 607–623, Jun. 1993.

[9] G. J. Sharpe, "Linear stability of planar premixed flames: Reactive Navier–Stokes equations with finite activation energy and arbitrary Lewis number," *Combustion Theory and Modelling*, vol. 7, no. 1, pp. 45–65, Mar. 2003.

[10] F. A. Williams, *Combustion theory: the fundamental theory of chemically reacting flow systems*, 2nd ed., ser. Combustion science and engineering series. Menlo Park, Calif: Benjamin/Cummings Pub. Co, 1985.

[11] W. Rakotoarison and M. I. Radulescu, "A dynamical system approach for solving the steady structure of high speed deflagrations," *Proceedings of the Combustion Institute*, Dec. 2022.

[12] S. A. E. G. Falle, "Self-similar jets," *Monthly Notices of the Royal Astronomical Society*, vol. 250, no. 3, pp. 581–596, Jun. 1991.

[13] S. A. E. G. Falle and S. S. Komissarov, "An upwind numerical scheme for relativistic hydrodynamics with a general equation of state," *Monthly Notices of the Royal Astronomical Society*, vol. 278, no. 2, pp. 586–602, Jan. 1996.

[14] S. A. E. G. Falle and J. R. Giddings, "Body capturing using adaptive cartesian grids," in *Baines, M.J., Morton, K.W. (Eds.), Numerical Methods for Fluid Dynamics*. Oxford University Press, 1993.

[15] D. H. Edwards and J. M. Morgan, "Instabilities in detonation waves near the limits of propagation," *Journal of Physics D: Applied Physics*, vol. 10, no. 17, p. 2377, Dec. 1977.

[16] A. Fecteau, "The Effects of Compressibility on the Propagation of Premixed Deflagration," Ph.D. dissertation, University of Ottawa, Ottawa, ON - Canada, 2019.

[17] M. Saif, W. Wang, A. Pekalski, M. Levin, and M. I. Radulescu, "Chapman–Jouguet deflagrations and their transition to detonation," *Proceedings of the Combustion Institute*, vol. 36, no. 2, pp. 2771–2779, 2017.

[18] B. Maxwell, A. Pekalski, and M. Radulescu, "Modelling of the transition of a turbulent shock-flame complex to detonation using the linear eddy model," *Combustion and Flame*, vol. 192, pp. 340–357, Jun. 2018.

[19] T. Jaravel, O. Dounia, Q. Malé, and O. Vermorel, "Deflagration to detonation transition in fast flames and tracking with chemical explosive mode analysis," *Proceedings of the Combustion Institute*, vol. 38, no. 3, pp. 3529–3536, Jan. 2021.

[20] W. Rakotoarison, B. Maxwell, A. Pekalski, and M. I. Radulescu, "Mechanism of flame acceleration and detonation transition from the interaction of a supersonic turbulent flame with an obstruction: Experiments in low pressure propane–oxygen mixtures," *Proceedings of the Combustion Institute*, vol. 37, no. 3, pp. 3713–3721, Jan. 2019.

[21] W. Rakotoarison, A. Pekalski, and M. I. Radulescu, "Detonation transition criteria from the interaction of supersonic shock-flame complexes with different shaped obstacles," *Journal of Loss Prevention in the Process Industries*, p. 103963, Feb. 2020.

[22] W. Rakotoarison, Y. Vilende, and M. Radulescu, "Model for CJ deflagrations in open ended tubes with varying vent ratios," in *Proceedings of the 27th International Colloquium on the Dynamics of Explosions and Reactive Systems*, Beijing, China, 2019.

[23] A. Y. Poludnenko, T. A. Gardiner, and E. S. Oran, "Spontaneous Transition of Turbulent Flames to Detonations in Unconfined Media," *Physical Review Letters*, vol. 107, no. 5, p. 054501, Jul. 2011.

[24] A. Y. Poludnenko, "Pulsating instability and self-acceleration of fast turbulent flames," *Physics of Fluids*, vol. 27, no. 1, p. 014106, Jan. 2015.

[25] A. Y. Poludnenko, J. Chambers, K. Ahmed, V. N. Gamezo, and B. D. Taylor, "A unified mechanism for unconfined deflagration-to-detonation transition in terrestrial chemical systems and type Ia supernovae," *Science*, vol. 366, no. 6465, Nov. 2019.

[26] M. I. Radulescu and J. Tang, "Nonlinear Dynamics of Self-Sustained Supersonic Reaction Waves: Fickett's Detonation Analogue," *Physical Review Letters*, vol. 107, no. 16, p. 164503, Oct. 2011, publisher: American Physical Society.