Modeling and Analysis of the Planar Jet-Stabilized Detonation Waves

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1 Introduction

The potential efficiency benefits of aerospace engines which use detonative combustion, such as the rotating detonation engine, has led in recent decades to active research efforts to understand the dynamics and structure of detonations. Despite significant progress, many open questions remain regarding the role of thermal non-equilibrium, real-gas effects, and boundary-layer interactions, to name a few. Such incomplete understanding of the physics of detonations manifests itself most visibly in a mismatch between experimental and numerical detonation cell sizes [1].

The jet-stabilized detonation wave (JSDW) (Fig. 1) represents a configuration which can provide a number of important practical advantages for studying detonations waves compared to the more traditional detonation channels [2–5]. In this configuration, a detonation is stabilized within an underexpanded reactive jet, in which the Mach disk formed by the jet serves as the leading shock of the detonation wave. Since such detonations are aerodynamically stabilized, they can be unconfined (at least at atmospheric conditions), providing easier optical access. Furthermore, instead of the detonation propagating through a tube at supersonic speeds, the JSDW is quasi-stationary, which allows for the observation of the detonation front over relatively long periods of time. The jet structure also provides increased control over the pre- and post-shock conditions, enabling the experiments to achieve burning behind the shock for a wide range of shock strengths, from strongly under-driven to over-driven conditions. Finally, the JSDW also provides a way to control the strength of non-equilibrium effects by varying the strength of the Mach shock and also by changing the degree of thermal non-equilibrium in the pre-shock jet flow.

Previous experimental attempts to establish standing normal detonation waves within a jet have generally been unsuccessful, with the fuel mixture either burning at, or near, the fuel injection site upstream of the shock, not burning at all, or burning after the shock in a decoupled manner that cannot be described as a detonation [2–5]. In part due to this lack of progress and concerns about the thermodynamic benefits of the use of standing normal detonation waves within an engine, research has moved more towards standing oblique detonation waves [6]. At the same time, more recent numerical work suggested that achieving a standing normal detonation within a jet may in fact be possible [7, 8].

One possible explanation for the lack of experimental observation of the JSDW is the lack of a theoretical model for predicting the jet conditions which are required to achieve a detonation for a given fuel mixture. If the jet stagnation temperature is too high, the mixture will burn before the shock; if it is

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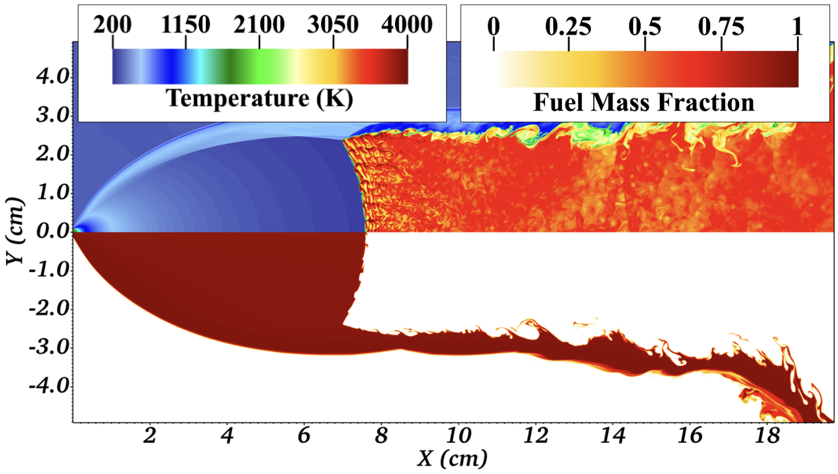

Figure 1: Instantaneous temperature (top) and fuel mass fraction (bottom) in a 2D planar jet-stabilized detonation.

too low, then it will not ignite after the shock. The range of stagnation conditions that will result in a detonation may be relatively small, or even nonexistent for some fuels, making jet-stabilized detonations difficult to achieve without the guidance of a predictive model. In this paper, a theoretical model for a simplified configuration of a 2D planar jet with single-step Arrhenius reaction kinetics is formulated and tested against numerical simulations.

2 Theoretical Framework for Reacting Underexpanded Jets

We seek to develop a framework which can accurately predict whether the fuel will burn upstream of the shock near the injector and also how the fuel will burn downstream of the shock. We make simplifying assumptions of a 2D planar jet, calorically perfect gas, and a single-step Arrhenius reaction model. A more detailed description will be presented in a separate paper.

The first step towards developing such a theoretical model of the underexpanded reacting jet is to create a centerline fluid trajectory based on a non-reacting jet simulation. Such trajectory provides the conditions which the jet material will encounter as it travels from the nozzle exit through the expansion barrel to the shock. For a constant specific heat ratio γ and molecular weight, such trajectories are self-similar for different nozzle conditions, thus only one base trajectory is needed to construct the inert trajectory for any set of stagnation conditions for a particular fuel. Reactions are then integrated over the entire trajectory to determine whether the fuel will ignite before reaching the shock.

If it is found that a fuel mixture at given stagnation conditions will not burn upstream of the shock, the next step is to characterize burning downstream of the shock. For this, the following quantity ξ is defined

$$\xi = \frac{D_m}{\Delta_i},$$

where D_m is the Mach disk diameter and Δ_i is the post-shock ignition length. This ratio compares the relevant hydrodynamic and chemical length scales, similar to a Damköhler number, Da, which compares the hydrodynamic and chemical time scales.

The Mach disk diameter, D_m, is calculated using a modified empirical relation similar in form to the expression developed by Avduevskii et al. [9]. To predict the post-shock ignition length, a 1D ZND steady-state solution is calculated using the static conditions immediately upstream of the Mach disk

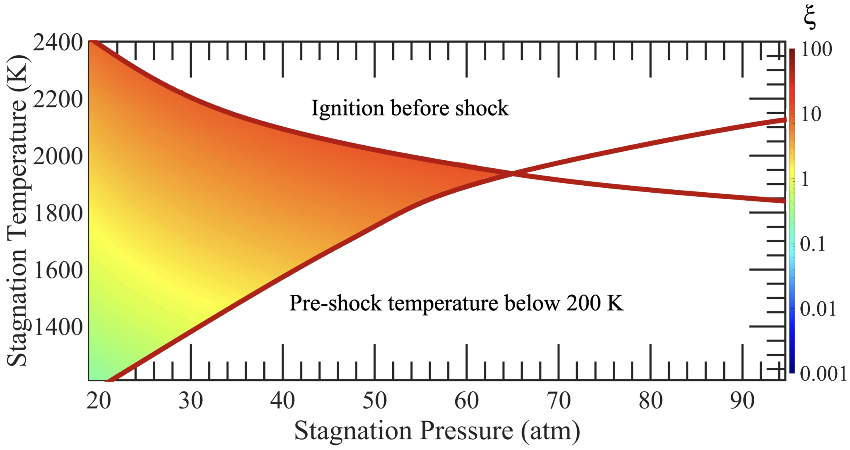

Figure 2: Example of the regime map of an underexpanded reacting jet.

as the initial condition, as well as the strength of the Mach shock. Since the jet trajectory has already been obtained, only the Mach disk position is needed in order to define where along that trajectory the initial state lies. Such Mach disk position is determined using another empirical relation [10]. The ZND solution provides the post-shock ignition length, which, along with the Mach disk diameter, gives the parameter ξ for a given mixture and stagnation conditions.

Results of such analysis can be visualized in a regime map, an example of which is shown in Fig. 2. The top white region represents conditions where the stagnation temperatures are too high and the fuel ignites before reaching the shock. White region on the bottom of the plot represents the flow regimes at which the pre-shock temperature drops below 200 K and thus simplifying thermodynamic assumptions made in the reacting jet model may depart significantly from reality. The colored region represents the range of operating conditions at which the fuel will not ignite or get too cold upstream of the shock. Within this region, higher (more red) or lower (more green) values of ξ suggest more or less vigorous burning behind the shock, respectively.

3 Numerical Method

To test the validity of the predictive theoretical framework described above, simulations were performed for a wide range of fuel properties and stagnation conditions by solving the unsteady, reactive, compressible Navier-Stokes equations with an ideal-gas equation of state. The massively parallel, adaptive mesh refinement code `Athena-RFX++` was used, which is a reacting-flow extension of the code `Athena++` [11]. The solver uses the 2^{nd}-order accurate van Leer predictor-corrector time integrator [12] with the piecewise-parabolic method (PPM) for spatial reconstruction [13]. Fluxes are calculated using the HLLC-ADC approximate Riemann solver [14] in order to minimize the carbuncle instability in normal grid-aligned shocks.

The numerical simulations are performed on an adaptively refined Cartesian grid comprised of a refined region containing the jet regions of interest and a large low-resolution surrounding region to avoid any spurious wave reflections coming from the outflow boundaries. The bottom boundary condition is symmetric (reflective, slip wall) so that only half of the jet is simulated to reduce the computational cost. The global domain is large enough to ensure that no waves created by the jet have time to travel to the right and top boundaries and reflect back to influence the jet structure before the simulation has completed. Zeroth-order extrapolated outflow boundary conditions were used along the top and right boundaries.

Along the left boundary, within the nozzle with exit radius r_e, a constant inflow boundary condition was

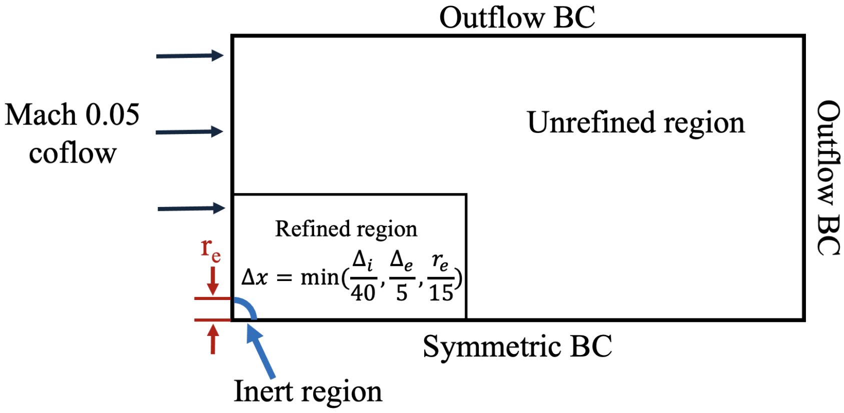

Figure 3: Schematic of the computational domain. The Δ_i and Δ_e are the induction length and exothermic pulse width based on the ZND solution.

set using the jet exit state with static pressure P_e, temperature T_e, x-velocity $v_{x,e}$, and fuel mass fraction $Y = 1$. Outside the nozzle along the left boundary, a coflow of air with Mach 0.05 was supplied. This coflow, which was also used in the prior numerical studies [7, 8], helps to stabilize the jet more quickly by slowly pushing the vortices formed outside of the jet boundary downstream. The overall schematic of the computational domain is shown in Fig. 3.

4 Simulation Results

Simulations performed over a wide range of mixture chemical properties and stagnation conditions revealed four different combustion regimes: non-reactive, pulsating, shock-induced combustion, and detonation.

For very low values of $\xi \lesssim 0.1$, the ignition length in the post-shock flow is too large for the mixture to ignite, and it either burns far downstream of the shock, or does not burn at all. For somewhat higher values of $0.1 \lesssim \xi \lesssim 1$, the jet is highly unstable, and its dynamics is dominated by a repeating cycle of over-driven detonations that push the Mach disk upstream followed by a detonation failure, when the Mach disk relaxes to its inert position (cf. Fig. 4).

Increasing the values of ξ further to $1 \lesssim \xi \lesssim 10$ results in a shock-induced combustion regime characterized by quasi-stable burning just downstream of the shock after some ignition delay (cf Fig. 5). This combustion mode was observed by Nicholls [3] and Rhodes et al. [4]. The shock-induced combustion mode is distinct from the detonative mode due to the lack of coupling between the shock and the reaction zone. Finally, once the value of ξ is high enough $\gtrsim 10$, combustion transitions into a detonative mode, in which the reaction zone becomes fully coupled to the shock and it produces the characteristic cellular structure (cf. Fig. 1).

5 Conclusions

We presented a comprehensive theoretical framework for predicting the behavior of a simplified 2D planar, underexpanded, reactive jet. This framework describes whether the fuel will ignite upstream of the shock and how the fuel will burn downstream of the shock, allowing for a more targeted choice of stagnation conditions in simulations and experiments required to achieve the desired combustion regime behind the jet Mach disk.

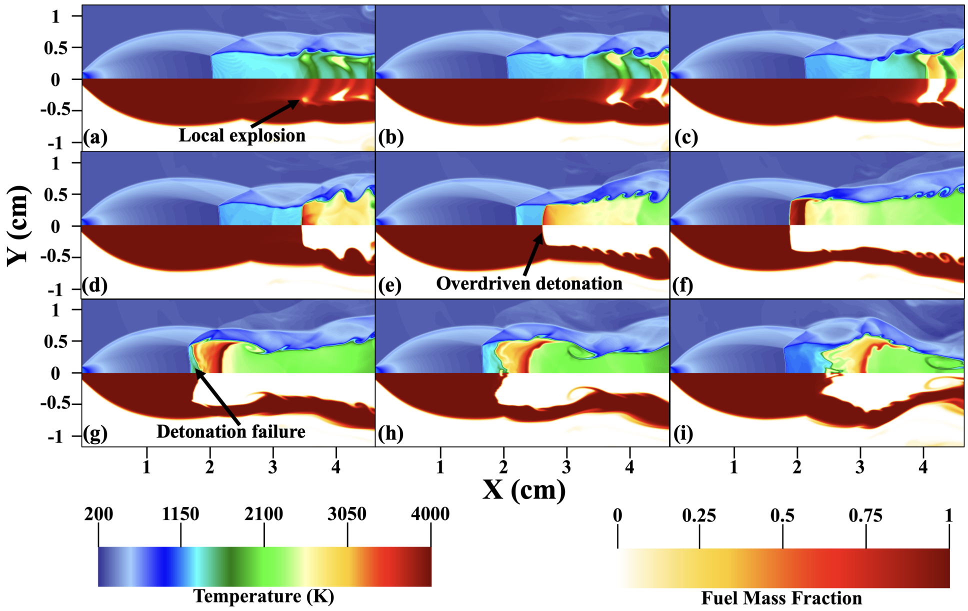

Figure 4: Evolution of temperature (top) and fuel mass fraction (bottom) in a pulsating case.

Simulations performed validate the framework over a range of chemical properties and stagnation conditions. Several burning regimes were observed that correspond to different ranges of the characteristic parameter ξ, with the highest values of ξ successfully predicting the formation of a jet-stabilized detonation wave.

In the future work, this model will be extended to more realistic 3D, axisymmetric jets with a realistic complex chemistry. The process of mixing must also be investigated. In this study, the fuel is assumed to be premixed at the nozzle exit, and the most optimal strategies for achieving such premixing must be determined for the design of the actual reacting jet experiments.

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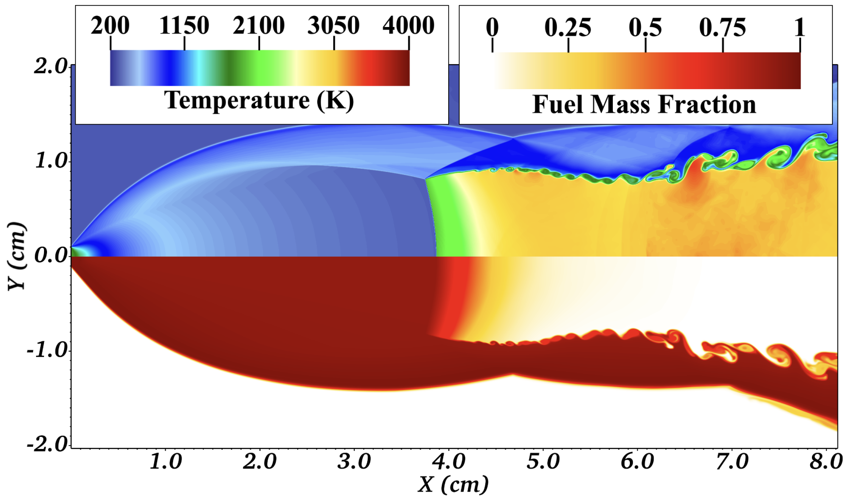

Figure 5: Instantaneous temperature (top) and fuel mass fraction (bottom) fields in a shock-induced combustion regime.

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