Model for Chapman-Jouguet deflagrations in open ended tubes with varying vent ratios

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1 Introduction

Turbulent deflagrations propagating in closed-ended tubes filled with obstacles are known to propagate at a speed given by the sound speed in the burned products, corresponding to a Chapman-Jouguet (CJ) deflagration [1]; this is the so-called *choking regime*. This is the limiting regime before a quasi-detonation can be achieved in more sensitive mixtures or tubes with a larger characteristic porosity length scale [2].

In deflagration to detonation transition (DDT) studies of non-sensitive mixtures, the critical burning velocity prior to rapid runaway to detonation waves was also found to be close to the CJ burning velocity, which is the maximal steady speed permissible [3–5]. CJ deflagrations propagating in tubes with a closed rear end were studied by Chue et al. [1]. They developed a quasi-steady, one-dimensional model that predicts the flame and shock speeds that satisfy the zero flow speed velocity owing to the rear boundary condition, forcing the CJ deflagration to propagate in the laboratory frame of reference at the sonic speed in the products. Different rear boundary conditions would give different absolute flame speeds and leading shock strengths. For example in the work of Saif et al., a similar model [6] was used to characterize the quasi-steady, one-dimensional flow resulting from the decoupling of a detonation through a perforated plate, that became a shock followed by a CJ deflagration. The latter was supported by steady over-expanded jets of burnt gases through the holes of the plate, leading to larger absolute flame speeds and stronger leading shocks than for the closed ended tube solution.

In the present study, we extend the CJ deflagration solution to deflagrations propagating in tubes with varying open area vent ratios. Other than finding direct application to fast flames propagating in tubes with open ends, the model is also expected to capture the fate of CJ deflagrations in different vented geometries, such as large scale tests of deflagrations where the sole confinement is provided by the congestion itself.

The present paper provides a gasdynamic model where the lead shock and CJ deflagrations are taken as discontinuities, where appropriate jump conditions may be applied, either using the perfect gas relations, or calculated numerically using equilibrium calculations and ideal gas thermochemical properties of the mixture. We formulate the problem of seeking the flame speed and lead shock strength of CJ deflagrations

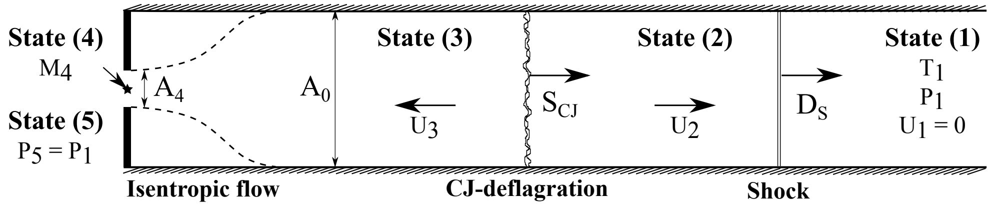


Figure 1: Schematic of the double discontinuity problem passed an obstruction.

propagating in tubes with ends of varying open areas, ranging from the closed end boundary condition [1] to the fully open area, and extending it to geometries using diverging nozzles accommodating further expansion of the product gases behind the CJ deflagration.

2 Model

The model configuration is presented in Figure 1. It consists in a tube of section area A_0, partially open at its back, providing an aperture with a section area A_4. The tube is filled with a gas at initial state (1). A shock propagating with a velocity D_s brings the flow to state (2). Thermodynamic properties and flow velocity are calculated using the shock-jump equations.

The shock is followed by a CJ deflagration propagating at the velocity S_{CJ} in the laboratory frame of reference, that brings the flow to state (3). Thermodynamic properties and flow velocity are calculated using the CJ deflagration jump conditions.

Due to the presence of the aperture downstream of the CJ deflagration, the flow is expanded isentropically to match the exit conditions at state (4), depending on the post-aperture state (5) where the pressure is fixed to match the initial pressure, i.e. $P_5 = P_1$.

The problem is solved by finding the shock speed that satisfies the boundary condition at the aperture, using numerical, iterative methods. Three cases are considered, and calculated in the following order:

1. From state (3), the flow reaches the choked state at the aperture, i.e. $M_4 = 1$ and is adapted to the atmosphere, i.e. $P_4 = P_5 = P_1$. In this case, the gas exits the tube through the aperture as a perfectly expanded sonic jet. This case is solved, first by iterating on the shock speed to satisfy the condition $P_4 = P_5$. It is done by calculating the state (3) for a given shock speed, then using the relation that links P_3 and P_4 in an isentropic flow, taking $M_4 = 1$. One could then deduce the associated aperture area section denoted A_4^* from the area - flow Mach number relation, as A_0, M_3 and $M_4 = 1$ are known.

2. Decreasing the area section of the aperture such that $A_4 < A_4^*$ keeps the flow choked at state (4), i.e., $M_4 = 1$, but increases the pressure P_4 such that $P_4 > P_5$. The gas is exiting the tube through the aperture as a choked, underexpanded jet. The entire flow is thus determined by iterating on the shock speed, to satisfy the only condition $M_4 = 1$. It is done by calculating the state (3) for a given shock speed, then using the area - flow Mach number relation between state (3) and state (4) to calculate M_4, as A_4/A_0 and M_3 are known.

3. Increasing the section of the aperture such that $A_4 > A_4^*$ keeps the pressure at state (4) being $P_4 = P_5$, but the flow is now subsonic, i.e., $M_4 < 1$. The gas is exiting the tube through the aperture as a

subsonic jet. The entire flow is thus determined by iterating on the shock speed, to satisfy the only condition $P_4 = P_5$. It is done by calculating the state (3) for a given shock speed, then using the area - flow Mach number relation and the isentropic relations between state (3) and state (4) to calculate M_4 and P_4, as A_4/A_0, M_3 and P_3 are known.

The set of jump conditions used so far could be derived in the perfect gas approximation with no changes of composition, provided the proper gas molecular mass, heat capacity ratio and heat of reaction. Jump conditions could also be calculated numerically, in the ideal gas approximation using ideal gas properties and equilibrium calculations to find the Chapman-Jouguet deflagration velocity and jump conditions. We have now developed this capability by extending the numerical methods developed by Shepherd and co-workers [7] with the help of the thermo-chemical toolbox Cantera [8]. Both perfect gas and ideal gas calculations are presented below.

3 Results

Results for the shock speed, shock overpressure and flame speed for a stoichiometric ethane - air mixture initially at 1 atmosphere and 300 K are presented in Fig. 2a, for both perfect gas (solid lines) and ideal gas with change of composition (dashed lines) approximations. The various quantities are plotted in terms of the ratio of open area to tube area A_4/A_0.

From this analysis, one could recognize two noteworthy conditions. The case where the section ratio $A_4/A_0 = 0$ corresponds to a tube with a closed end. The results recover those of Chue et al. [1] for a closed end tube. The deflagration speed in the absolute frame exceeds 1000 m/s and drives a stronger shock with an overpressure of appoximately 9 - 12.5 bar.

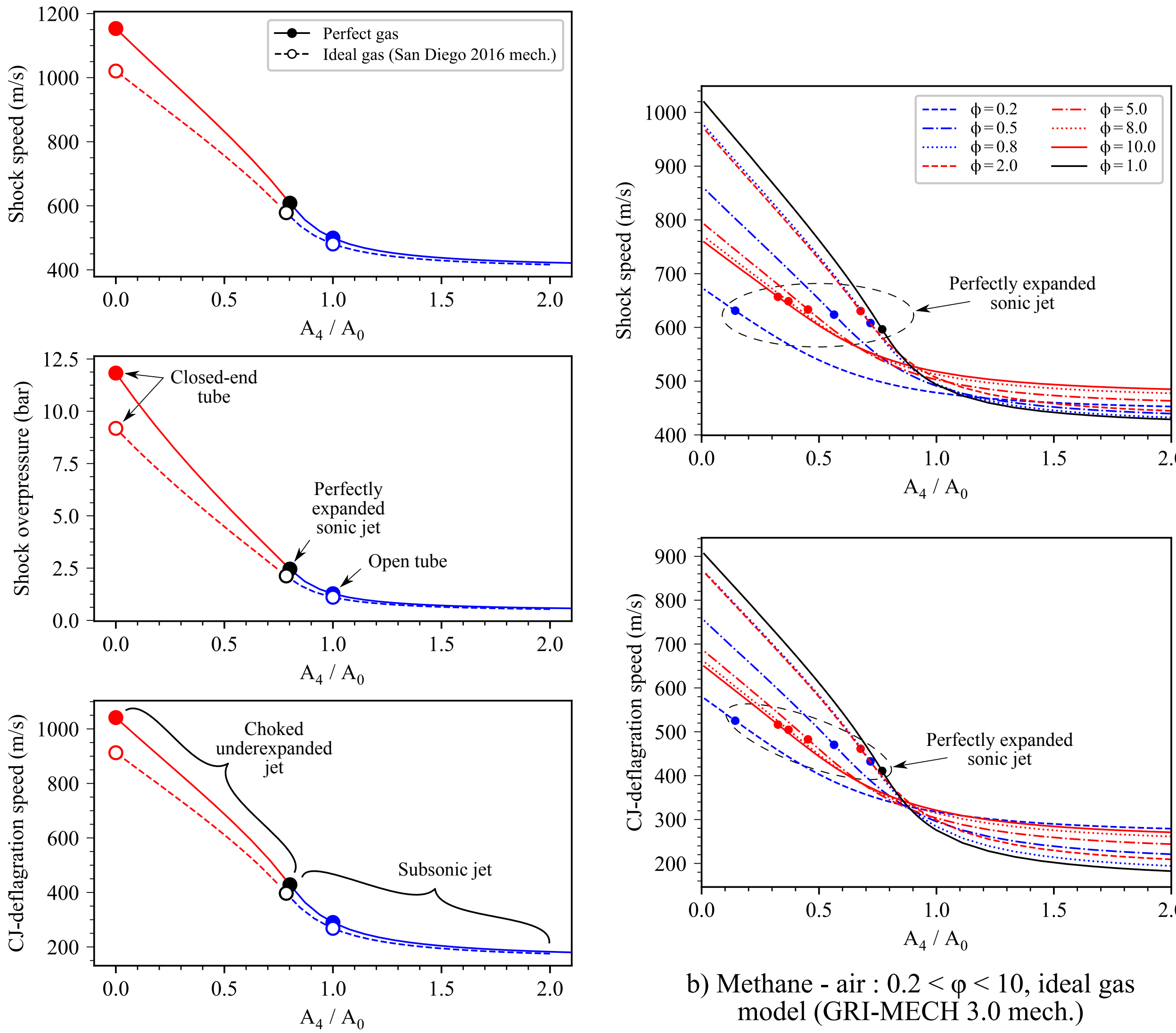
The case where the section ratio $A_4/A_0 = 1$ corresponds to an open-ended tube venting to the atmosphere. In this case, due to the efficient venting of the products to the rear, the absolute flame speed is only approximately 300 m/s and generates a weak shock with negligible overpressure.

In between these two extremes, the shock and flame speeds, as well as the pressure of the explosion are a strong function of the area ratio A_4/A_0. Smaller exhaust areas impede the de-pressurization of the combustion products and hence drive faster flames and lead shocks.

Our results have also been extended to area ratios $A_4/A_0 > 1$, corresponding to scenarios where the open area is larger than the tube itself. Slower deflagrations with negligible shocks are obtained.

Results for the shock speed and flame speed for methane - air mixtures initially at 1 atmosphere and 300 K with equivalence ratio ϕ ranging between 0.2 and 10 are presented in Fig. 2b, in the ideal gas with change of composition approximation. The various quantities are plotted in terms of the ratio of open area to tube area A_4/A_0, and show the same trends as in Fig. 2a.

An interesting implication of the present results pertains to the speed of turbulent deflagrations that can be attained in vented large scale experiments, such as those compiled recently by Pekalski et al. [9]. In such tests, deflagrations cannot be supported by a closed confinement, and the product gases motion is solely impeded by the congestion itself. Indeed, the maximum deflagration speed prior to transition to detonation was found to depend on congestion blockage, and was significantly lower than the sound speed in the burned gases. Future work should be devoted to testing the present model to turbulent flame propagation in vented explosions with rear and side relief.



a) Stochiometric ethane - air

b) Methane - air : 0.2 < φ < 10, ideal gas model (GRI-MECH 3.0 mech.)

Figure 2: a) Shock speed, shock overpressure and CJ deflagration speed in a fixed frame of reference as a function of the section ratio A_4/A_0, for stoichiometric ethane - air mixture at initial pressure and temperature 1 atmosphere, 300 K. b) Shock-Mach number and CJ deflagration speed in a fixed frame of reference as a function of the section ratio A_4/A_0 for methane - air mixtures with equivalence ratio ϕ ranging between 0.2 and 10, at initial pressure and temperature 1 atmosphere, 300 K.

Limitations of this model are related to the assumptions done on the uniformity of state (2), the isentropic flow occurring between states (3) and (4), and the fact that the jump conditions across the flame is directly determined by the thermodynamics of flames propagating with burning velocities equal to the CJ deflagration ones, with no mention on how such velocities are reached. In practice, flames that reach the CJ deflagration regime are turbulent, and propagate in tubes with series of obstructions or rough walls. This would imply supplementary considerations on the shock propagation, that would be different than in the case of propagation in unobstructed channels with smooth walls, as well as including non-uniformities in state (2) and non-isentropic flow between states (3) and (4). Such considerations shall be accounted in further extensions of this model, in order to characterize shock - CJ deflagration complexes in more realistic configurations.

4 Conclusion

The present paper generalized the analysis of Chue et al. [1] for CJ deflagrations propagating in tubes by allowing the tube end to assume different open area ratios. It was found that while the flame speed was given by the sound speed in the burned products for a closed end tube ($\sim$ 1000 m/s), this speed is a strong function of the vent ratio. For an open ended tube, the absolute flame speed drops to approximately 300 m/s and generates negligible overpressures. At intermediate vent ratios, a continuous range of flame speeds can be expected. The results obtained indicate that DDT criteria formulated in terms of a critical flame speed in vented explosions [9] are likely a very strong function of the amount of venting allowed by the congested geometry or other pressure relief devices.

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