On the Predicability of Weakly Confined Gaseous Detonations Using the Straight Streamline Approximation

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1 Introduction

The fast energy deposition in the reaction zone of gaseous detonations has motivated their application in novel propulsion systems [1], such as Rotating Detonation Engines (RDEs) [2, 3] and Pulse Detonation Engines (PDEs) [4]. Transverse detonations in rotating detonation engines are weakly confined by fresh injected gases on one side and by combustion products on the other. This weak confinement of a detonation permits lateral flow divergence in the reaction zone and controls the detonation deficits and, ultimately, the detonation limits. This problem of detonation propagating in layers weakly confined by an inert gas has attracted much work since the work of Dabora [5]. Reynaud et al. provide a summary of the state of the art in computations and experiments [6].

Progress in modelling of this phenomenon was restricted mostly to condensed-phase detonations, with the pioneering work of Wood and Kirkwood [7] and Bdzil and Stewart's Detonation Shock Dynamics (DSD) [8]. The DSD work is meant as a rational multi-scale approach to treating the problem exploiting certain limits in simple reaction models. However, an approximate model has been suggested by Watt et al. [9], which makes *à priori* a straight streamline approximation (SSA) in the reaction zone. In each stream tube, the equations of motion are integrated separately, with regular conditions at the sonic locus providing the constraints at the shock. The last stream tube and its interaction with the confiner closes the problem. The problem is defined by a series of ODEs along each streamtube, which can easily be integrated for arbitrarily complex chemistry. The entire reaction zone structure can be obtained, along with the front sock curvature, velocity deficit and dependence on confining gas. Although approximate, Watt and his co-workers have shown that the SSA model can be very accurate in predicting numerical solutions and DSD predictions for simple pressure-dependent kinetics relevant to condensed-phase detonations. Watt's SSA model also offers the opportunity of incorporating more sophisticated chemistry models for integration along each stream-tubes.

In the present study, we wish to determine how the SSA model performs for Arrhenius kinetics with parameters relevant for gas-phase detonations. We thus perform calculations using the SSA model and compare with the recent numerical results of Reynaud et al. [6] and Mi et al. [10]. While the agreement will be shown to be very good for weakly unstable detonations, the departure of the model for more unstable detonations can be quantitatively reconciled by the effect of the cellular structure in lengthening the global reaction zone structure of detonations.

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2 Model

Watt et al. developed a mathematical model based on the fluid-streamline approach of reactive gas flow across the detonation front to study the dynamics of condensed-phase explosives [9]. The model is based on adapting the steady reactive Euler equations in streamline coordinates(ψ, y) and assumes straight streamlines. Fig. 1 shows the setup. With the appropriate boundary conditions at the shock, the equations governing the velocity, and rate of burning of reactants, on a particular streamline, under the approximation of straight streamlines, are given by equations (1) and (2). The initial pressure, density and half-reaction zone length of the ZND solution are chosen to non-dimensionalize the system.

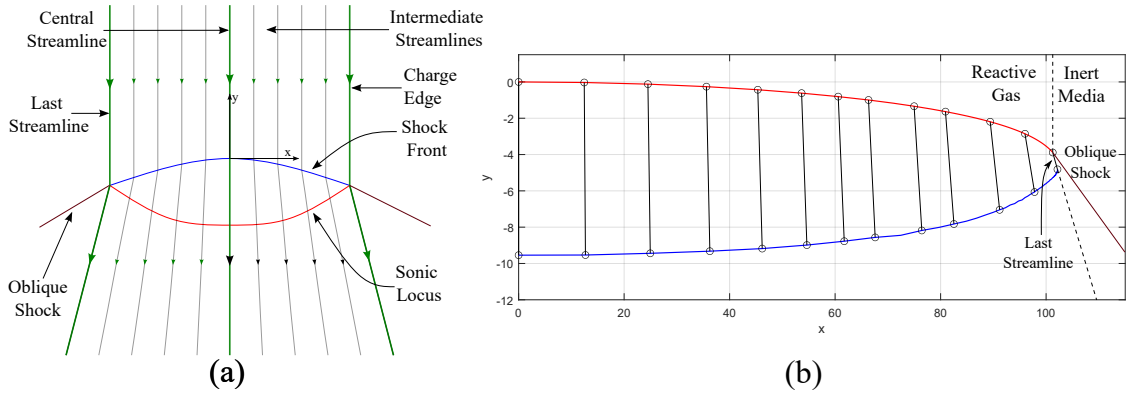

Figure 1: SSA Model - (a) Schematic of lateral flow divergence of steady detonation as defined in Straight Streamline Model. (b) Detonation front (red), sonic locus (blue), and streamlines from SSA model for $D/D_{CJ} = 0.98$ for $E_a/RT_0 = 10, \gamma = 1.333, Q/RT_0 = 23.81$.

$$\frac{\partial v}{\partial y} = \frac{\left(\frac{\partial x}{\partial \psi}\right)^{-1} c^2 v \frac{\partial^2 x}{\partial y \partial \psi} - (\gamma - 1) Q W}{\left[v^2 \left(1 + \left(\frac{\partial x}{\partial y}\right)^2\right) - c^2\right]} \tag{1}$$

$$\frac{\partial \lambda}{\partial y} = \frac{W}{v} \tag{2}$$

The equations are coupled with the rate law for energy deposition W. In the present study, we adopt a one-step Arrhenius law.

The governing equations, along with initial conditions, evaluated using normal shock-jump conditions, were integrated numerically until the generalized Chapman-Jouguet condition was met at the sonic locus at the end of each streamline. For a given detonation speed, the equations are integrated from the charge axis for increasing ψ until the streamline deflection angle is reached to match the physical boundary condition at the inert layer. While for strong confinement, this involves a shock polar analysis for the transmitted shock into the inert layer, for weak confinement, the edge boundary condition is given by the maximum streamline divergence. The latter boundary condition is adopted here to address the computations of Reynaud et al. and Mi et al. A detailed description of the model is given in Cartright's PhD thesis [11]. This integration procedure determines the entire reaction zone structure and the thickness of explosive h corresponding with the assumed velocity. A schematic of the structure of detonation as obtained from the SSA model is showed in Fig. 1. The term $\frac{dx}{dy}$ corresponds to the slope of the streamline, and terms $\frac{dx}{d\phi}$ and $\frac{d^2x}{dyd\phi}$ represent effective flow divergence present in the reaction-zone structure of the detonation.

3 Results and Discussion

The comparison of the Straight Streamline Model with numerical simulations of detonation propagating in reactive gas confined by an inert gas, existing in literature, is presented here. The first set of comparisons is made with the numerical computation results of Reynaud, and his peers [6]. For all the simulations performed by Reynaud, Q/RT_0 is fixed at 23.81 and γ = 1.333. Four different values of the reduced activation energy E_a/RT_0 were used - 10, 20, 30 and 38.23. The initial thermodynamic properties are identical for reactive charge and inert media.

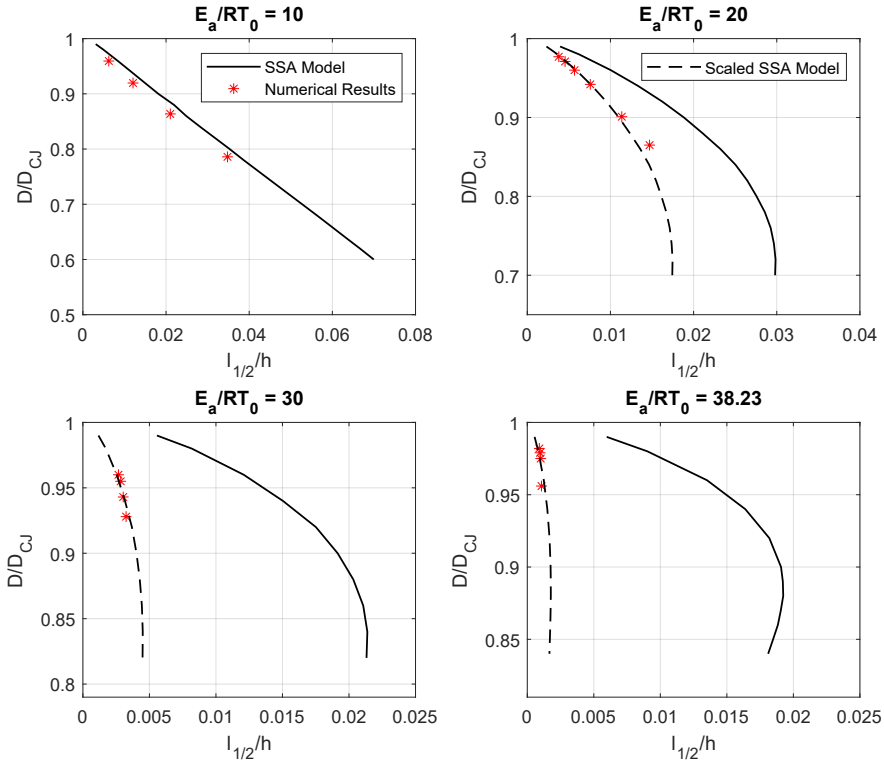

Figure 2: Comparision of Straight Streamline Model with Reynaud's Simulation [6].

Fig. 2 shows the prediction of the velocity of detonation for gaseous detonation confined by compressible inert layer by straight streamline model. For $E_a/RT_0 = 10$, the straight streamline model is in excellent agreement with numerical simulations. However, SSA Model is unable to find the critical height for this case. As the activation energy increases, this agreement starts to deteriorate as evident from Fig. 2. This discrepancy is due to the delayed burning of reactants for high-activation energy cases and the presence of cellular structure.

Similarly, the model is compared against the results of Mi's numerical simulation [10], as shown in Fig. 3. Three different values of E_a/RT_0 are considered here - 10, 20 and 30. The non-dimensionalized heat release $Q/RT_0 = 50$ and ratio of specific heats γ = 1.2. As shown in Fig. 3, SSA model is in near-perfect agreement for $E_a/RT_0 = 10$. Thus, SSA model can predict the velocity of detonations for lower activation energies, but fails for higher activation activation energies.

The difference between calculations experiments are due to the cellular structure of detonations, non-accounted for in the macro-scopic kinetic model used. Indeed, Reynaud has measured the average reaction zone structure of each cellular detonation and compared it qualitatively with the corresponding

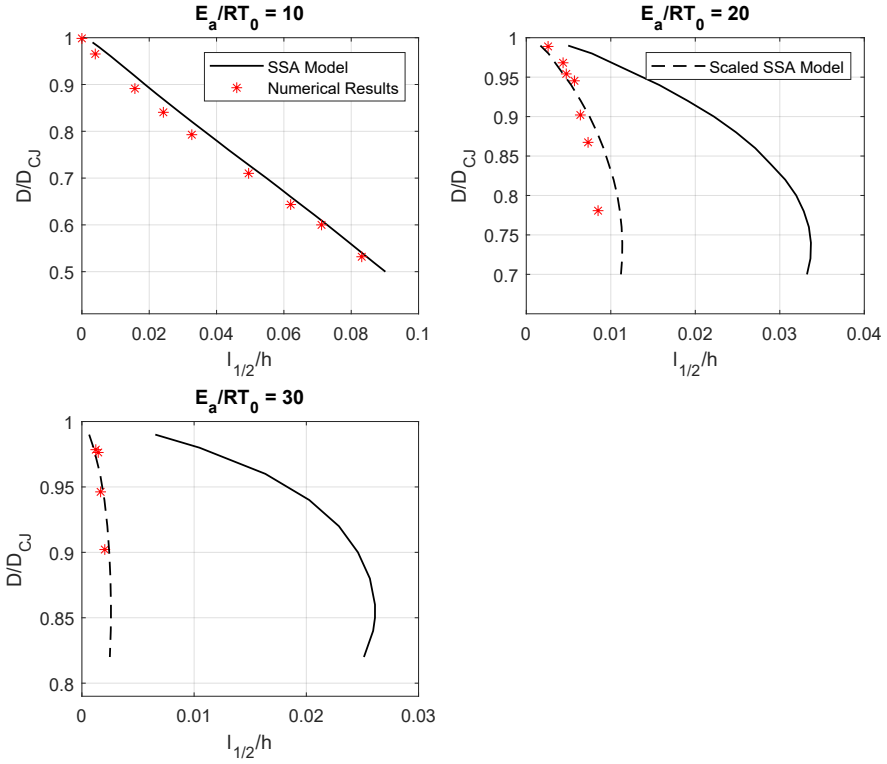

Figure 3: Comparision of Straight Streamline Model with Mi's numerical calculations [10].

laminar structure. We have analyzed their data and extracted an effective coefficient G by which the cellular structure slows down the global rate of reactant depletion. Note that G is the effective scaling of reaction-zone structure as observed by comparing the reaction concentration profiles for the Wood-Kirkwood model and numerical computations as provided in [6] for $E_a/RT_0 = 10, 20 \,\&\, 30$. This coefficient is shown in Fig. 4 in terms of the reduced activation energy by the shock temperature, i.e. E_a/RT_{VN}. It shows an increasing exponential trend.

Interestingly, the SSA model can be made to agree if the kinetics were slowed down by a constant factor $G1$ for each set of activation energies very comparable to G. These re-scaled results are shown as dotted lines in Fig. 2 and 3. Fig. 4 also shows the variation of the scale parameter in terms of the reduced activation energy by the shock temperature. i.e. E_a/RT_{VN}, which is different in Reynaud's and Mi's calculations. The data collapse well onto a single curve, with an exponential dependence on activation energy.

The good correspondence between the two scaling factors strongly suggests that the SSA model would continue to work well in predicting the detonation response if the effective kinetic slow-down due to the cellular structure was modeled correctly. More importantly, it also suggests that a hydrodynamic description is a meaningful approach to model cellular detonations with losses [12–14].

A physical model incorporating the exponential dependence of ignition delay on temperature and reduced activation energy is in development to account for the cellular structure of the detonation to address the reaction-zone lengthening present in irregular detonations. The results of this model will be communicated at the conference.

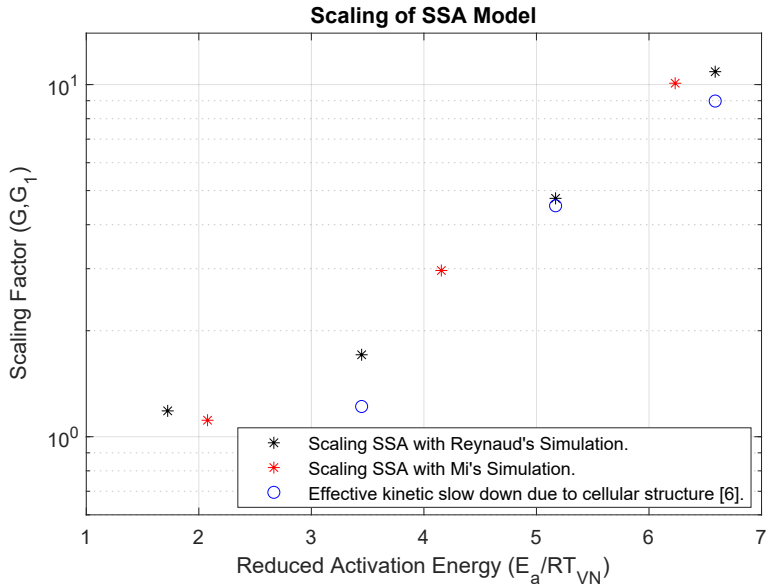

Figure 4: Scaling of SSA Model with Numerical simulations.

References

[1] J. E. Shepherd, "Detonation in gases," *Proceedings of the Combustion Institute*, vol. 32, no. 1, pp. 83–98, 2009.

[2] D. Schwer and K. Kailasanath, "Numerical study of the effects of engine size n rotating detonation engines," in *49th AIAA aerospace sciences meeting including the new horizons forum and aerospace exposition*, 2011, p. 581.

[3] F. K. Lu and E. M. Braun, "Rotating detonation wave propulsion: experimental challenges, modeling, and engine concepts," *Journal of Propulsion and Power*, vol. 30, no. 5, pp. 1125–1142, 2014.

[4] G. D. Roy, S. M. Frolov, D. W. Netzer, and A. A. Borisov, "High-speed deflagration and detonation: Fundamentals and control. international colloquium on control and detonation processes held in moscow, russia on july 4-7, 2000," ELEX-KM PUBLISHERS MOSCOW (RUSSIA), Tech. Rep., 2001.

[5] E. K. Dabora, J. Nicholls, and R. Morrison, "The influence of a compressible boundary on the propagation of gaseous detonations," in *Symposium (International) on Combustion*, vol. 10, no. 1. Elsevier, 1965, pp. 817–830.

[6] M. Reynaud, F. Virot, and A. Chinnayya, "A computational study of the interaction of gaseous detonations with a compressible layer," *Physics of Fluids*, vol. 29, no. 5, p. 056101, 2017.

[7] W. W. Wood and J. G. Kirkwood, "Diameter effect in condensed explosives. the relation between velocity and radius of curvature of the detonation wave," *The Journal of Chemical Physics*, vol. 22, no. 11, pp. 1920–1924, 1954.

[8] J. B. Bdzil and D. S. Stewart, "Modeling two-dimensional detonations with detonation shock dynamics," *Physics of Fluids A: Fluid Dynamics*, vol. 1, no. 7, pp. 1261–1267, 1989.

[9] S. D. Watt, G. J. Sharpe, S. A. Falle, and M. Braithwaite, "A streamline approach to two-dimensional steady non-ideal detonation: the straight streamline approximation," *Journal of Engineering Mathematics*, vol. 75, no. 1, pp. 1–14, 2012.

[10] X. Mi, A. Higgins, C. Kiyanda, H. Ng, and N. Nikiforakis, "Effect of spatial inhomogeneities on detonation propagation with yielding confinement," *Shock Waves*, vol. 28, no. 5, pp. 993–1009, 2018.

[11] M. Cartwright, "Modelling of non-ideal steady detonations," Ph.D. dissertation, University of Leeds, 2016.

[12] M. I. Radulescu, G. J. Sharpe, C. K. Law, and J. H. S. Lee, "The hydrodynamic structure of unstable cellular detonations," *Journal of Fluid Mechanics*, vol. 580, pp. 31–81, 2007.

[13] M. I. Radulescu and B. Borzou, "Dynamics of detonations with a constant mean flow divergence," *Journal of Fluid Mechanics*, vol. 845, pp. 346–377, 2018.

[14] Q. Xiao and M. I. Radulescu, "Role of instability on the limits of laterally strained detonation waves," *Combustion and Flame*, vol. 220, pp. 410–428, 2020.