# Method of Characteristics Analysis of Gaseous Detonations Bounded by an Inert Gas

Robert Fievisohn and Kenneth Yu
University of Maryland
College Park, Maryland

## 1 Introduction

Detonation waves bounded by an inert gas have traditionally been studied as an analog to the confinement problem in solid explosives or to characterize vapor cloud and free jet explosions. [1–4] A similar flow field is also observed in Rotating Detonation Engines (RDEs). [5] By studying the relatively simple problem of a detonation bounded by an inert gas, researchers may gain a better understanding of the physical processes occurring within an RDE.

This research focuses on modeling the bulk fluid flow of a detonation bounded by an inert gas in the wave-fixed reference frame accurately and rapidly. Major flow features such as the detonation wave, oblique shock, and contact surface are modeled analytically. Once these parameters are known, a shock-fitted numerical solution is initialized. Since the analysis occurs in the steady wave-fixed reference frame and the flow is supersonic; a method of characteristics solution is chosen for accuracy and speed.

Early work on detonations bounded by an inert gas on one side was done by Sommers and Morrison. [1] Two analytical models for the system were proposed to calculate the oblique shock and slip line angles. Dabora, Nicholls, and Morrison analyzed the same system to determine the effect of inert boundaries on the wave propagation velocity and detonatability limits. [2] Additional work was also conducted by Sichel and Foster to generate the ground impulse of a passing detonation wave in a vapor cloud. [3] In that paper, a method of characteristics solution was initialized from a centered expansion fan. The solution was only carried out until the expansion fan reflected off the bottom boundary in order to generate a ground pressure distribution. The current work extends this solution to the rest of the flowfield and also examines different ways to analytically model the detonation wave.

## 2 Theory

### Idealized Flow Structure

An idealized description of the detonation bounded by an inert gas system is shown in Fig. 1. Sommers and Morrison put forth two methods for calculating the oblique shock, interface, and centered expansion properties. [1] The first method is based on 2D shock-expansion theory. Following Fig. 1, if the post-detonation conditions are provided; $D$ and $P_{e_2}$ are known. Since $P_{e_3} = P_{i_2}$, there now only exist 3 unknowns: $\beta$, $\theta$, and $P_{e_3}$ (or $P_{i_2}$).

Note that subscript $i$ represents the inert gas and subscript $e$ represents the explosive gas. The following three equations describing the oblique shock, expansion fan, and pressure matching conditions can be used to iteratively solve for the unknowns. The first is the theta-beta-Mach relation:

$$\tan\theta = 2\cot\beta\left[\frac{M_{i_1}^2\sin^2\beta - 1}{M_{i_1}^2(\gamma_i + \cos 2\beta) + 2}\right]. \tag{1}$$

The second describes a Prandtl-Meyer expansion:

$$\theta = \sqrt{\frac{\gamma_{e_2}+1}{\gamma_{e_2}-1}}\tan^{-1}\sqrt{\frac{\gamma_{e_2}-1}{\gamma_{e_2}+1}(M_{e_3}^2 - 1)} - \tan^{-1}\sqrt{M_{e_3}^2 - 1}. \tag{2}$$

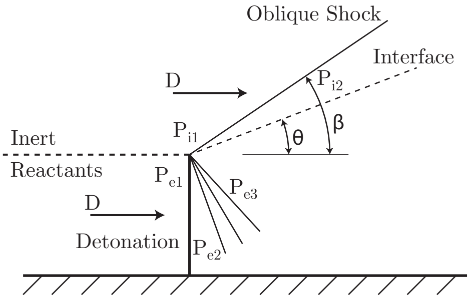


Figure 1: Idealized flow structure for a detonation wave bounded by an inert gas.

Lastly, the pressure matching condition is given by

$$\frac{P_{i_1}}{P_{e_1}}\left[1 + \frac{2\gamma_i}{\gamma_i + 1}(M_{i_1}^2\sin^2\beta - 1)\right] = \frac{P_{e_2}}{P_{e_1}}\left[\frac{\frac{\gamma_{e_2}+1}{2}}{1 + \frac{\gamma_{e_2}-1}{2}M_{e_3}^2}\right]^{\frac{\gamma_{e_2}}{(\gamma_{e_2}-1)}}. \tag{3}$$

The second method for calculating the major flow features uses a 1D shock tube analogy where the post-detonation gas is the driver gas and the inert gas is the driven gas. Using the shock tube analogy, the pressure across the oblique shock wave may be calculated implicitly using

$$\frac{P_{e_2}}{P_{i_1}} = \frac{P_{i_2}}{P_{i_1}}\left\{1 - \frac{(\gamma_{e_2}-1)(a_{i_1}/a_{e_2})(P_{i_2}/P_{i_1} - 1)}{\sqrt{2\gamma_i[2\gamma_i + (\gamma_i + 1)(P_{i_2}/P_{i_1} - 1)]}}\right\}^{-2\gamma_{e_2}/(\gamma_{e_2}-1)}. \tag{4}$$

Once the pressure across the oblique shock has been estimated, the vertical component of velocity along the interface may be found using

$$u_p = \frac{a_{i_1}}{\gamma_i}\left(\frac{P_{i_2}}{P_{i_1}} - 1\right)\left(\frac{\frac{2\gamma_i}{\gamma_i+1}}{\frac{P_{i_2}}{P_{i_1}} + \frac{\gamma_i-1}{\gamma_i+1}}\right)^{1/2} \tag{5}$$

where $u_p$ is the piston or vertical component of the interface velocity. The slip line angle may now be found as

$$\tan\theta = \frac{u_p}{D}. \tag{6}$$

There are two possible ways of computing the oblique shock angle within the shock tube analogy. The first is to calculate the vertical shock velocity as

$$W = a_{i_1}\sqrt{\frac{\gamma_i + 1}{2\gamma_i}\left(\frac{P_{i_2}}{P_{i_1}} - 1\right) + 1} \tag{7}$$

and finding the shock angle with

$$\tan\beta = \frac{W}{D}. \tag{8}$$

The second is to follow Dabora, Nicholls, and Morrison [2] and use wave refraction relations which reduce to

$$\sin\beta = \frac{W}{D}. \tag{9}$$

This basically states that the pressure jump and resulting velocity from the shock tube relations are the conditions normal to shock. It will be shown that for inert gases with low acoustic impedance ratios, Eq. (9) more closely follows the results from shock-expansion theory.

Note that the above relations do not assume that the initial pressures in the inert and explosive are the same. It is highly unlikely that this would be the case for vapor cloud or free jet explosions but it is possible that the axial pressure gradient in an RDE may be approximated with different pressures in the reactant inflow and bounding detonation products.

The main flow structures of this system (oblique shock and slip line angles) have been shown to be a function of the ratio of acoustic impedances between the inert and explosive gases [1] defined as

$$\frac{Z_{i_1}}{Z_{e_1}} = \frac{\rho_{i_1} a_{i_1}}{\rho_{i_1} a_{e_1}}. \tag{10}$$

If there is a difference in pressure across the initial explosive/inert interface, the flow structures have been shown to be a function of what Dabora, Nicholls, and Morrison call the density parameter [2] defined as

$$\bar{\rho} = \sqrt{\frac{\rho_{i_1} \gamma_i}{\rho_{e_1} \gamma_{e_1}}}. \tag{11}$$

If $P_{i_1} = P_{e_1}$, then the density parameter reduces to the ratio of acoustic impedances. Figures 2 and 3 show the variation in oblique shock and slip line angle versus the ratio of the acoustic impedances. A simple, constant $\gamma$, constant molecular weight model for hydrogen-air mixtures developed by Gamezo, Ogawa, and Oran was used to generate the plots. [6] The acoustic impedance in the explosive was held constant and the acoustic impedance in the inert was varied by changing the temperature. Dashed lines highlight a low temperature solution and an approximate RDE solution. The low temperature solution (300K inert gas) is more representative of vapor cloud and free jet explosions. The approximate RDE solution is found by assuming that the temperature of the bounding gas is found by isentropically expanding the detonation products to the initial explosive mixture pressure:

$$\frac{T_{i_1}}{T_{e_2}} = \left(\frac{P_{i_1}}{P_{e_2}}\right)^{(\gamma_{e_2}-1)/\gamma_{e_2}}. \tag{12}$$

Also included in Fig. 3 is the maximum oblique shock angle according to the theta-beta-Mach relations. When the solution intersects this line, the shock-expansion theory breaks down since the oblique shock

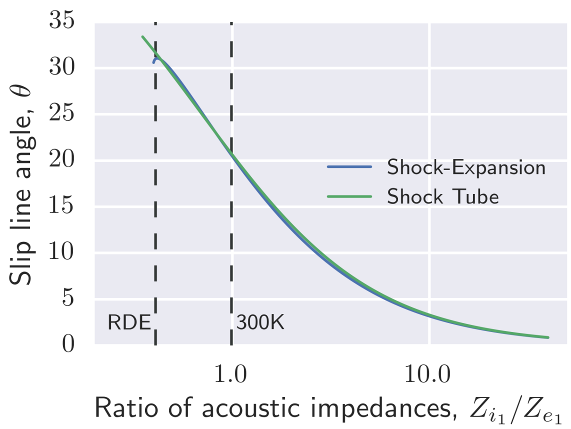


Figure 2: Slip line or interface angle versus the ratio of acoustic impedances.

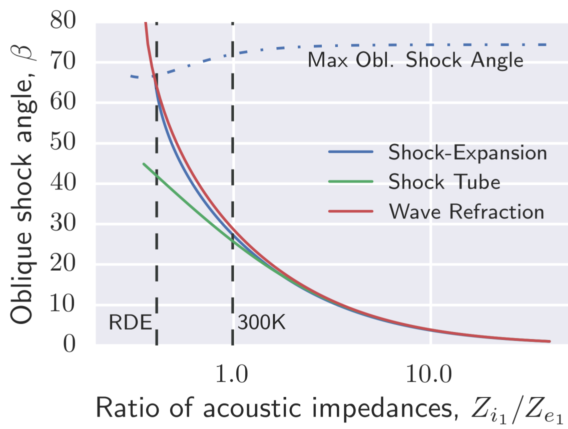


Figure 3: Oblique shock angle versus the ratio of acoustic impedances.

would now become a detached shock. It is important to note that the RDE solution is very close to where the shock will detach. This may have implications when attempting to analytically model the flow structures in an RDE. One advantage of the shock tube theory is that it will still give an approximate answer even for very low acoustic impedances in the inert.

Experimental evidence has shown that the idealized flow model satisfactorily predicts observed shock and slip line angles. [1, 2] The majority of the experimental work was performed with low temperature air as the bounding inert. Experiments with helium as the inert gas were also conducted and more closely resemble the flow angles observed in RDE experiments and simulations; however, additional experimental work on this system with low acoustic impedance inert gases would be extremely valuable to the RDE research community.

## Method of Characteristics

The method of characteristics is a method for solving hyperbolic partial differential equations. The steady, two-dimensional Euler equations are hyperbolic for flow velocities greater than Mach 1. Since the analysis occurs in the steady wave-fixed frame and the flow behind the oblique shock and detonation is supersonic, this system is ideally suited for the method of characteristics. The formulation, unit processes, and marching techniques for steady two-dimensional isentropic supersonic flow presented by Zucrow and Hoffman is used. [7]

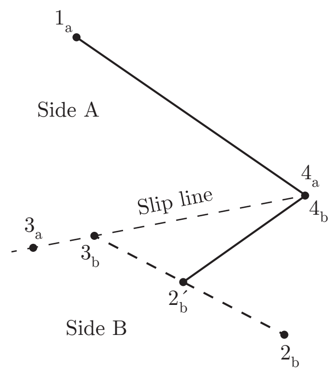


Figure 4: Illustration of slip line unit process.

To model the flow behind a detonation bounded by an inert, the solution is broken up into two domains. The first is the post-detonation flow. This section is initialized from the centered expansion fan at the top of the detonation wave. The solution is then marched following a manner similar to an internal nozzle flow; however, the top boundary of the domain is a slip line and not a solid wall. The second domain is the post-oblique shock flow. An initial value line is defined starting at the first point where the leading characteristic from the post-detonation flow intersects the slip line. The marching technique for this domain is similar to a supersonic external flow field with the exception that the bottom boundary is now a slip line and not a solid wall. Since a unit process for handling a slip line with supersonic flow on both sides for rotational flow could not be found in the literature, a new unit process was developed.

The unit process for a slip line in rotational flow is illustrated in Fig. 4. In this picture, point $4_a$ is the new point being solved for. The solution process is similar to Thompson's unit process for a slip line in irrotational flow but with modifications for rotational flow and changing conditions on side B. [8] The first step is to estimate the pressure at point $4_a$ and determine the resulting flow angle and position. The next step is to apply this angle and position to point $4_b$. The conditions at point $4_b$ are solved using the indirect wall method shown in Zucrow and Hoffman. [7] Point $2_b'$ is interpolated between points $2_b$ and $3_b$ to find the correct Mach line for point $4_b$. Once the pressure at point $4_b$ is calculated, this is used to update the assumed pressure at point $4_a$. This process is repeated until the pressures at points $4_a$ and $4_b$ match.

## Detonation Modeling

This idealized model assumes the detonation is planar, infinitely thin, and therefore governed by ideal Chapman-Jouget theory. Since the wave is of finite height, loss mechanisms such as friction, heat

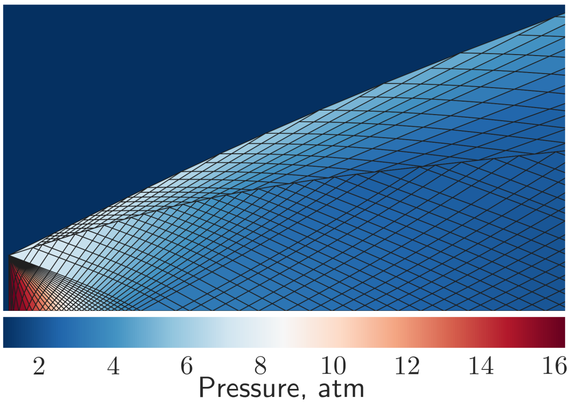


Figure 5: MOC solution for stoichiometric $H_2$-air detonation bounded by air at standard conditions.

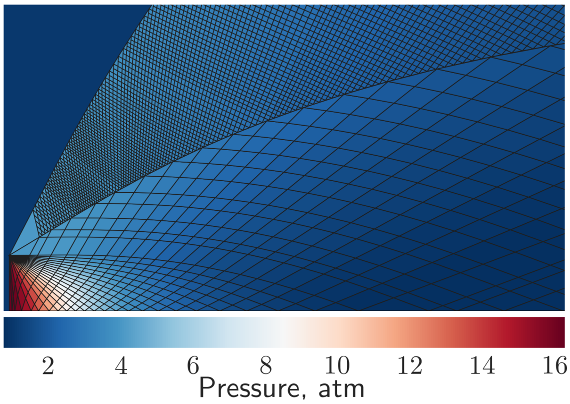


Figure 6: MOC solution for stoichiometric $H_2$-air detonation bounded by isentropically expanded detonation produts.

conduction, and area divergence through the reaction zone will affect wave propagation. These effects may be modeled using the quasi-1D, reactive Euler equations. [9] It should also be noted that any area divergence through the reaction zone implies that the wave is curved. [9] Curvature based models would account for velocity deficits, non-ideal post-detonation pressures and temperatures, and differences in the observed shock and slip line angles. These effects are explored within the field of Detonation Shock Dynamics (DSD). [10]

The current work is more focused on developing the method of characteristics solution procedure based on analytically based boundary conditions. Future work incorporating more realistic detonation models to include non-ideal effects and curvature is planned. Lastly, the effect of the true multi-dimensional structure on this system needs to be examined.

## 3 Results and Discussion

The full method of characteristics solutions are given in Figs. 5 and 6. Figure 5 is a stoichiometric hydrogen-air detonation bounded by air at 300K. Figure 6 is similar but bounded by hot, isentropically expanded detonation products to approximate the expected behavior in an RDE. Note the difference in the oblique shock and slip line angles. These solutions run very quickly since the analytical treatment of the oblique shock and detonation removes the requirement to resolve these features numerically. Also, the equations being solved are the true steady state Euler equations so iterating to a converged solution is not required. A frozen 2-$\gamma$ model also simplifies the equation set to be solved. Lastly, less resolution is required due to the low dissipative nature of the method of characteristics; however, the MOC solution also has its drawbacks. Chiefly, the lack of flexibility. A MOC solution requires knowing where any discontinuities are beforehand and treating them analytically. Any new discontinuities are generally ignored with the hope that it does not make that much of a difference in the final solution.

This solution methodology is similar to Detonation Shock Dynamics (DSD) wherein a propagation model for a detonation and it's interactions with a boundary are used as boundary conditions for a numerical simulation. Unlike DSD, this model is focused on gaseous detonations bounded by inert gases rather than confined solid explosives. Curvature is important for the propagation of solid explosives and a significant portion of DSD theory is devoted to modeling this effect. Future work on this model will also incorporate results from DSD theory to include curvature effects; however, additional work may be necessary to include the effect of the prominent multi-dimensional wave structure observed in gaseous detonations. Additionally, detonation-boundary interactions in DSD theory will also be incorporated to help model cases where the oblique shock wave has detached and a secondary shock reflects back into the detonation products.

A detonation bounded by an inert gas and the internal flow in an RDE have similar flow features. The simple model developed here can compute the bulk fluid flow in a detonation bounded by an inert gas and is the first step towards developing a quick, simple model for parametric studies of RDE performance. Studying detonations bounded by an inert gas provides a simpler system to test theories and models before applying them to RDE flow fields. Future work on the development of this model include curvature effects, examining vortex development along the slip line, and the inclusion of chemically reacting flow. Applying the model to RDE flows is already underway with the development of an inflow boundary condition and periodic boundary conditions. It is hoped that the RDE version of this model will give an accurate estimate of performance to allow quick parametric studies of RDE geometries.

## References

[1] W. P. Sommers and R. B. Morrison, "Simulation of condensed-explosive detonation phenomena with gases," *The Physics of Fluids*, vol. 5, no. 2, pp. 241–248, 1962.

[2] 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.

[3] M. Sichel and J. Foster, "The ground impulse generated by a plane fuel-air explosion with side relief," *Acta Astronautica*, vol. 6, no. 3, pp. 243–256, 1979.

[4] T. Fujiwara and S.-i. Tsuge, "Quasi-onedimensional analysis of gaseous free detonations," *Journal of the Physical Society of Japan*, vol. 33, no. 1, pp. 237–241, 1972.

[5] 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.

[6] V. N. Gamezo, T. Ogawa, and E. S. Oran, "Numerical simulations of flame propagation and ddt in obstructed channels filled with hydrogen–air mixture," *Proceedings of the Combustion Institute*, vol. 31, no. 2, pp. 2463–2471, 2007.

[7] M. J. Zucrow and J. D. Hoffman, *Gas dynamics. Volume 2-Multidimensional flow*. New York: John Wiley and Sons, Inc., 1977.

[8] P. A. Thompson, *Compressible-fluid dynamics*. New York: McGraw-Hill, 1971.

[9] A. Higgins, "Steady one-dimensional detonations," in *Shock Waves Science and Technology Library, Vol. 6*. Springer, 2012, pp. 33–105.

[10] J. B. Bdzil and D. S. Stewart, "Theory of detonation shock dynamics," in *Shock Waves Science and Technology Library, Vol. 6*. Springer, 2012, pp. 373–453.