One-dimensional modeling of gaseous detonation in a packed bed of solid spheres

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1 Introduction

The problem of detonation in systems with heat and momentum losses was, for the fist time, considered by Zel'dovich in his fundamental paper of 1940 [1]. The losses were modeled within the one-dimensional framework for the problem of gaseous detonation in a tube. The momentum loss was due to the friction of the gas with the tube walls and the heat loss due to both the work done by the friction losses and the heat transfer between the gas and the wall. In particular, Zel'dovich estimated the magnitude of the velocity deficit incurred due to the losses and provided a qualitative discussion of the physical mechanisms for such deficits. It is of relevance to our present work to also point out that in [1], Zel'dovich indicates a possibility of the flow reversal in the reaction zone. That is, in the laboratory frame of reference, the flow of the gas can, over some region of space, be in the direction opposite to that of the lead shock. Even though such a solution was presented in [1, 2], no detailed study of the conditions or mechanisms has been carried out.

The problem of detonation with losses has been revisited subsequently by many researchers, including Zel'dovich himself with co-workers [3, 4], as well as many others [5–8]. The principal theoretical reasons for revisiting the problem are the difficulties associated with the existence of multiple steady-state solutions for a given set of parameters, describing the explosive mixture and the losses. A natural question to ask is: Which of these steady solutions occur in practice and how are they related to observations [9]? This question is, in particular, closely related to that of stability of the possible steady solutions and remains largely open.

In [3], the authors calculated the effects of heat and momentum losses on the detonation in rough tubes. The detonation-velocity deficits have been calculated for several gaseous mixtures as a function of the friction factor. Only the high-velocity branch was calculated. Even though the cases of the flow reversal were computed, they were not investigated in any detail. However, the authors remark that the convective heat losses alone were insufficient in causing the flow reversal, since such losses vanish with the velocity. This observation is in contrast to our present finding that, in a closely related problem, the flow reversal is possible even if only the convective heat transfer is accounted for. We also find that the flow reversal in our model is impossible in self-sustained detonations when only the momentum loss is included.

In modeling such complex flows as the gaseous detonation in a porous medium, an important question is: To what extent is it possible to use a simplified one-dimensional model? In other words, what are

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the limits of such models? In this work, our goal is to attempt to reproduce theoretically the observed variety of detonation regimes by using a single-step global reaction model within the one-dimensional reactive-flow framework.

2 One-dimensional modeling

We consider the flow of a compressible reacting ideal gas in a packed bed of solid particles. The particles are assumed immobile and non-reacting. Their only role is to absorb the momentum and thermal energy of the detonating gas through friction and heat transfer. We note, however, that the friction plays a dual role as it leads to not only the momentum loss, but also to heating. The gaseous detonation is described by a simplified model consisting of the reactive Euler equations with a one-step reaction, $A \to B$, proceeding at the Arrhenius rate, $\omega = k\left(1-\lambda\right)\exp\left(-E/pv\right)$. Here λ is the reaction-progress variable (the fraction of the released chemical energy, which goes from $\lambda = 0$ at the shock to $\lambda = 1$ at the end of the reaction), E is the activation energy, p is pressure, $v = 1/\rho$ is the specific volume, ρ is density, and k is the pre-exponential rate factor. The gas internal energy is given by the equation of state of a perfect gas, $e_i = pv/\left(\gamma-1\right)$, where γ is the constant ratio of specific heats. The governing reactive Euler equations accounting for the losses of momentum and energy are

$$\rho_t + (\rho u)_x = 0, \tag{1}$$

$$u_t + u u_x = -\frac{1}{\rho} p_x - \frac{f}{\rho\phi}, \tag{2}$$

$$p_t + u p_x + \gamma p u_x = \left(\gamma-1\right) Q\rho\omega + \left(\gamma-1\right)\left(\frac{uf-h}{\phi}\right), \tag{3}$$

$$\lambda_t + u\lambda_x = \omega. \tag{4}$$

Here u is the gas velocity and f is the drag force described by the formula [10]

$$f = A_s\rho\left(b_1 + \frac{b_2}{Re}\right)u|u|, \tag{5}$$

where $A_s = 6\left(1-\phi\right)/d$, d is the particle diameter, $Re = d_p|u|/\nu$ is the Reynolds number (where $d_p = \frac{2\phi}{3(1-\phi)}d$), ϕ is the porosity (the fraction of space occupied by the gas), and b_1, b_2 are numerical parameters.

The energy equation (3) contains contributions due to: the chemical energy release (the first term, where Q is the heat release), the work done by the friction forces (the second term, involving uf), and the heat transfer between the gas and the particles (the last term, proportional to h). The heat exchange rate is assumed to be given by [10]

$$h = A_s\alpha_s\left(T - T_s\right), \tag{6}$$

where the particle temperature is denoted by T_s and is assumed to be constant. The gas temperature is given by the ideal gas law, $T = pvW/R$, where R is the universal gas constant and W is the molecular mass of the gas. The heat conduction coefficient α_s is calculated from $\alpha_s = \lambda_g Nu/d_p$, where $Nu = a_1 + a_2 Re^m$ is the Nusselt number. We note that there is some discrepancy in the literature as to the form of the energy equation (cf. [1,6,7] vs [2,3]). Our formulation is similar to that of [2,3].

We assume the Reynolds number to be sufficiently large, so that we can take $b_1 = 0.75$ and $b_2 = 0$. For the Nusselt number we take $a_1 = 0$, $a_2 = 0.0425$, and $m = 1$. It is important to note that in this approximation both f and h are equal to zero when $u = 0$. While generally speaking, it is incorrect to assume the vanishing heat conduction in a quiescent gas, the high gas velocity in the reaction zone justifies this assumption. The velocity vanishes, in most cases, only in the far field, where the reaction has ended. This is not so in the presence of the flow reversal within the reaction zone, however, but then the vanishing of u occurs at a single point, so that the corresponding vanishing of h at that point is unlikely to have any appreciable effect on the flow.

In conservation form, the momentum, energy, and the reaction equations can be written as

$$(\rho u)_t + \left(p + \rho u^2\right)_x = -\frac{f}{\phi}. \tag{7}$$

$$(\rho e)_t + (\rho u\,(e + pv))_x = -\frac{h}{\phi}, \tag{8}$$

$$(\rho \lambda)_t + (\rho u \lambda)_x = \rho \omega, \tag{9}$$

where $e = e_i + u^2/2 - \lambda Q = pv/\left(\gamma - 1\right) + u^2/2 - \lambda Q$. The Rankine-Hugoniot conditions have the same form as for the ideal case (i.e. the case without losses). Using the following rescaling (subscript a denotes the ambient state): $\hat{\rho} = \rho/\rho_a$, $\hat{p} = p/p_a$, $\hat{u} = u\sqrt{\rho_a/p_a}$, $\hat{x} = x/l_{1/2}$, $\hat{t} = t\sqrt{\rho_a/p_a}/l_{1/2}$, $\hat{E} = E/p_a v_a$, $\hat{Q} = Q/p_a v_a$, $\hat{T} = TR/p_a v_a W = \hat{p}/\hat{\rho}$, $\hat{D} = D\sqrt{\rho_a/p_a}$, the governing equations can be non-dimensionalized. The equations however retain their form wherein the dimensionless loss terms become (dropping the hats after the rescaling):

$$f = c_f \rho |u| u, \qquad c_f = 6b_1\left(1 - \phi\right) \cdot \frac{l_{1/2}}{d}, \tag{10}$$

$$h = c_h |u| (T - 1), \quad c_h = \frac{9a_2(1-\phi)^2}{\phi} \cdot \frac{l_t l_{1/2}}{l_v d}. \tag{11}$$

Here $l_t = \lambda_g W/R\sqrt{p_a \rho_a}$, $l_v = \nu/\sqrt{p_a/\rho_a}$, and $l_{1/2}$ is the half-length of the reaction zone (the distance from the shock to the point where $\lambda = 0.5$). The dimensionless coefficients c_f and c_h, which are now just two numbers measuring the effects of the momentum and heat losses, respectively, depend on the ratios of various length scales characteristic of the relevant transport processes. For c_f, it is the ratio of the length of the reaction zone and the particle diameter. For c_h, it is a non-trivial combination of four length scales: the viscous scale, l_v, the thermal scale, l_t, the reaction scale, $l_{1/2}$, and the particle diameter, d. We note however that $c_h/c_f = \left[1.5a_2\left(1 - \phi\right)/b_1\phi\right]\,(l_t/l_v)$, which is independent of the reaction or the particle diameter.

3 Steady-state structure

In addition to the usual set of parameters of the ideal detonation (i.e. E, Q, γ), we now have two additional parameters measuring the contributions of the momentum and heat losses, which affect the structure of the steady-state solutions. While the literature contains a number of results in this direction [1, 3–5, 7, 9], a comprehensive study is lacking, especially when both heat and momentum losses are present and when the stability question is concerned.

We seek traveling-wave solutions of the governing equations as $\mathbf{U} = \begin{pmatrix} \rho & u & p & \lambda \end{pmatrix}^T = \mathbf{U}\left(\xi\right)$ where $\xi = x - Dt$ and D is the detonation velocity. The continuity equation yields $\rho\left(D - u\right) = \rho_a D$, which is the only conserved quantity in the presence of losses. The governing equations can be written as

$$(\mathbf{A} - D\mathbf{I})\mathbf{U}' = \mathbf{G}, \tag{12}$$

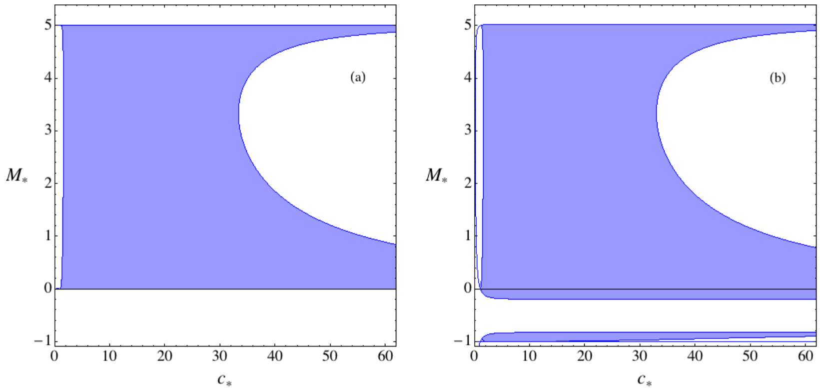

Figure 1: The domains of existence of the sonic locus in the plane of the Mach number, $M_* = u_*/c_*$, and the sound speed, c_*, at the sonic point: (a) with only the momentum loss and (b) with both momentum and heat losses. The boundaries of the shaded regions are given by $\lambda_* = 0$ and $\lambda_* = 1$.

where $\mathbf{G} = \begin{pmatrix} 0 & F & G & \omega \end{pmatrix}^T$, $\mathbf{A}$ is the coefficient matrix, $\mathbf{I}$ is the unit matrix, and $F = -f/\rho\phi$, $H = (\gamma-1)Q\rho\omega + (\gamma-1)\,(uf-h)\,/\rho\phi$. The acoustic eigenvalues of $\mathbf{A}$ are $s_1 = u+c$ and $s_2 = u-c$, where $c = \sqrt{\gamma p/\rho}$ is the sound speed. The corresponding left eigenvectors are $\mathbf{l}_1 = \left(0, 1, \frac{c}{\gamma p}, 0\right)$ and $\mathbf{l}_2 = \left(0, 1, -\frac{c}{\gamma p}, 0\right)$. Multiplying (12) from left by $\mathbf{l}_1$, we obtain $(s_1 - D)(u' + \frac{c}{\gamma p}p') = F + \frac{c}{\gamma p}H$. Multiplying by $\mathbf{l}_2$, we obtain $(s_2 - D)(u' - \frac{c}{\gamma p}p') = F - \frac{c}{\gamma p}H$. From these equations, it follows that

$$u' = \frac{1}{2}\frac{F + \frac{c}{\gamma p}H}{u+c-D} + \frac{1}{2}\frac{F - \frac{c}{\gamma p}H}{u-c-D}, \tag{13}$$

$$p' = \frac{\gamma p}{2c}\frac{F + \frac{c}{\gamma p}H}{u+c-D} - \frac{\gamma p}{2c}\frac{F - \frac{c}{\gamma p}H}{u-c-D}. \tag{14}$$

We look for solutions of (13)–(14) that smoothly pass through a sonic point, $\xi = \xi_*$, where $u+c-D = 0$ and $F + cH/\gamma p = 0$. Denote all quantities at ξ_* by a subscript $*$. Then the following two conditions must be satisfied at ξ_* :

$$\frac{(\gamma-1)\,c_*}{\gamma p_*}\left(Q\rho_*\omega_* + \frac{u_* f_* - h_*}{\phi}\right) - \frac{f_*}{\rho_*\phi} = 0, \tag{15}$$

$$u_* + c_* - D = 0. \tag{16}$$

Equation (16) is easy to solve for the detonation speed D using $c_* = \sqrt{\gamma p_*/\rho_*} = \sqrt{\gamma p_*\,(D-u_*)\,/\rho_a D}$; its only positive root is then $D = \frac{1}{2}\left(u_* + \sqrt{u_*^2 + 4\gamma p_*}\right)$. Equation (15) yields

$$\lambda_* = 1 - \exp\left(\frac{E}{p_* v_*}\right)\frac{\gamma p_*}{kc_*(\gamma-1)Q\rho_*}\left(\frac{f_*}{\gamma\rho_*} + (\gamma-1)\frac{c_*}{\gamma p_*}\frac{h_* - u_* f_*}{\phi}\right). \tag{17}$$

The problem for the steady-state structure in the λ variable (obtained from (13)–(14) using $d\xi = \frac{u-D}{\omega}d\lambda$) has the following form:

$$\frac{du}{d\lambda} = g_1\left(u, p, \lambda; \{D, c_f, c_h\}\right), \quad \frac{dp}{d\lambda} = g_2\left(u, p, \lambda; \{D, c_f, c_h\}\right), \tag{18}$$

with the initial conditions at the shock, $u(0) = \frac{2(D^2-\gamma)}{(\gamma+1)D}$ and $p(0) = 1 + \frac{2(D^2-\gamma)}{\gamma+1}$.

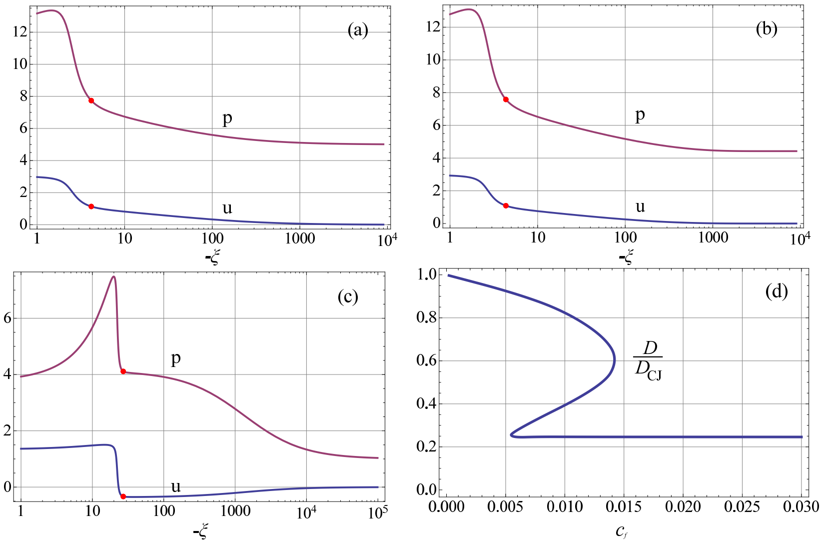

Figure 2: The velocity and pressure profiles when: (a) $c_f = 0.01$, $c_h = 0$; (b-c) $c_f = 0.01$, $c_h = 0.01$; (b) corresponds to the upper branch and (c) to the middle branch of $D - c_f$ curve in (d); (d) D/D_{CJ} vs c_f at $c_h = 0.01$. The red points on the curves in (a-c) indicate the sonic locus.

The solutions $u(\lambda)$, $p(\lambda)$ of (18) must be found together with the detonation speed D. For any given set of parameters (e.g. c_f, c_h), the solutions of (18) will satisfy the sonic conditions (15)–(16) only at particular values of D. Thus one must search for D numerically in order to obtain the complete solution of the problem. The sonic point ξ_* is of a saddle type, which makes integration from the shock toward the end of the reaction zone technically difficult. We therefore integrate from the sonic point both to the shock and to the point where $u = 0$, where both the momentum and heat losses vanish and all unknown functions in $\mathbf{U}$ become constant.

An initial guess for $u_*,\ p_*$ is needed to start the integration. Here and in all the computations below, we use $\gamma = 1.2$, $E = Q = 20$, and $k = 261.84$. If only the momentum losses are present ($c_f \neq 0,\ c_h = 0$), we find the domain of the possible existence of the sonic point as shown in Fig. 1(a). The shaded area is bounded by $\lambda_* = 0$ and $\lambda_* = 1$ from (17) and is plotted in terms of the Mach number $M_* = u_*/c_*$ and the sound speed c_*. Note that the flow velocity at the sonic point can only be positive. This domain is scanned to find the solutions of (17). The computed solution profiles in ξ variable are shown in Fig. 2(a). Here $\xi = 0$ is the position of the shock and $\xi = -\infty$ is the end of the computed region, where $u = 0$ and $\lambda = 1$. One notable feature, in contrast to the ideal detonation case, is the increase of pressure shortly behind the shock, which is due to the resistance of the solid particles to the gas expansion.

When both momentum and heat losses are present, i.e. $c_f \neq 0$ and $c_h \neq 0$, the region in the M_*-c_* plane where a sonic point can exist is significantly more complicated, see Fig. 1(b). The most important new feature is the appearance of a new region where the particle velocity at the sonic point can be negative. That is, around the sonic point there can be a region of flow in the negative direction in the laboratory frame. Eventually, far from the shock, the flow velocity returns to zero. Such flow reversal is found to be possible, in this model, only in the presence of heat losses. Corresponding solution profiles are shown in Fig. 2(b-c). Behind the sonic point the velocity tends to zero at infinity.

By fixing $c_h = 0.01$, we computed the dependence of the detonation velocity as a function of the friction factor, c_f, as shown in Fig. 2(d). The characteristic turning-point behavior is seen. In experiments, the top and bottom branches are observed (e.g. [9]), while the middle branch is not, apparently due to the latter solution's instability. The solution profiles shown in Fig. 2(b-c) differ in several important respects. The characteristic length scales in the reaction zones are vastly different in the two cases and so is the behavior as $\xi \to -\infty$. In both cases, the velocity tends to zero as $\xi \to -\infty$, in (c) going through the intermediate negative phase, but in Fig. 2(b), in contrast to (c), the pressure does not tend to 1. This is explained by the fact that the heat loss term has vanished due to the vanishing velocity. The present model does not account for conductive heat losses and therefore the gas remains hot in the far field in this particular case. Apparently, the gas has stopped too fast for the cooling to be able to bring down the gas temperature to sufficiently low levels.

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