A Study of Detonation Evolution and Structure for a Model of Compressible Two-Phase Reactive Flow

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Abstract

A two-phase model of heterogeneous explosives, due to Baer and Nunziato, is examined computationally by a new numerical approach that is a modification of the standard Godunov scheme. The approach generates well-resolved and accurate solutions economically, and treats rationally the nozzling terms that render the otherwise hyperbolic model incapable of a conservative representation. A broad range of the parameter space is investigated and two possible structures of steady, planar detonations are identified, along with subregions of the parameter space where they exist. The transient processes subsequent to impact by a low-speed piston are studied in detail, for a variety of cases, to describe the transition from a compaction wave to one or the other of the two steady detonation waves. The findings are compared with existing computational results.

1 Introduction

High-energy, condensed-phase explosives are heterogeneous composites with a complex microstructure, consisting of grains of the crystalline explosive embedded in a plastic binder matrix. Since well-resolved computations at the grain scale are impractical at the present time, current mathematical models of reactive flow in explosives are designed to apply at the macroscale and as such, involve some level of homogenization. The simplest approach that takes explicit account of the heterogeneity treats the material as a two-phase mixture of coexisting and interacting continua, consisting of grains of the reacting solid and the gaseous products of combustion. This approach is exemplified in the work of Baer and Nunziato (hereafter referred to as BN) who also provide an extensive historical review [1]. Contemporaneous studies by Butler and Krier [2] and the later papers by Powers, Stewart and Krier [3, 4] also deserve mention.

The fundamental assumption underlying the two-phase approach is that each phase is in local thermodynamic equilibrium. Nonequilibrium interactions do occur between the phases, and are driven by the processes of compaction, drag, heat transfer and reaction. The mathematical description consists of a system of hyperbolic partial differential equations representing the balance of mass, momentum and energy for each phase together with a compaction law and a saturation constraint. While mass, momentum and energy are conserved for the mixture, these quantities are not conserved separately for each phase. The exchange processes appear in the model as source terms. It is noteworthy that some of the source terms are proportional to the gradient of the volume fraction of the solid phase. These so-called nozzling terms arise in the modeling process and describe the exchange of momentum and energy between phases due to a change in the cross-sectional area of a virtual stream tube of the gas phase. The presence of these terms prevents the governing hyperbolic system from being expressed in conservation form, and this has important consequences in the devising of a suitable computational strategy.

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While the general form of the two-phase approach is accepted in the literature, several variations of the original, BN model have appeared; see, for example, the work by Gonthier and Powers [5, 6] and by Saurel and coworkers [7, 8]. These models differ primarily in the choices made for the equations of state and the form of the exchange source terms. For example the Powers-Stewart-Krier model, proposed in [3] and subjected to analysis and computation in [4, 5, 6], does not contain the aforementioned nozzling terms. In recent work the BN model has been re-examined by Bdzil et al [9] who have suggested some modifications. Asymptotic reductions of the model in the realistic limits of large drag and rapid compaction have also been considered [10, 11]; see also [12].

Upon application of a mechanical or thermal stimulus of sufficient strength, the solid explosive may detonate. A principal goal of a reactive-flow model is to predict how and when the detonation forms, what its structure is, how it responds to disturbances, and how a propagating detonation can fail. The present work focuses on the evolution and structure of planar detonation for the two-phase BN model, as modified in [9]. This is done by considering the response of the explosive to a low-speed piston impact. The result is not a prompt initiation to detonation, but rather, a slower buildup to it. Highly-resolved numerical solutions of the governing equations are computed to determine the evolutionary process leading up to, and the ultimate structure of, the steady detonation wave. To be sure, this task has been considered previously by Baer and Nunziato [1], and by Gonthier and Powers [6]. For a particular data set, and by using the method-of-lines approach, Baer and Nunziato [1] gave an account of the evolutionary process and identified the mechanisms of transition in some detail. Additional results were presented in their study for a less porous explosive and for a range of compaction viscosities. Gonthier and Powers [6] considered a variant of the model that did not include the nozzling terms. Their results, based on the Godunov approach, were also confined to a particular parameter set, with the structure of the steady wave as the primary focus. A related study in which the solid phase was considered incompressible was carried out by Papalexandris [13], including two-dimensional simulations.

The present study adds two new aspects. First, we present a new numerical procedure that treats the nonconservative source terms in a rational way and results in highly accurate and well-resolved solutions. Second, we examine a broad region of the parameter space to assess how the various parameters appearing in the source terms of the model affect both the steady structure and the evolutionary process. This information provides a quantitative understanding of the role of the various source terms, thus aiding the process of calibration with experiments.

The focus is on parameters that determine the relative strength of reaction and the rates of the relaxation processes of compaction, drag and heat transfer. We find that while the choice of parameters does not significantly affect the speed of the steady detonation, it strongly influences, in general, the run to detonation and the structure of the steady wave. Figure 1 shows representative profiles of the solid volume fraction for the two basic steady detonation structures found in our study. The structure on the left, which we call a compaction-led detonation, is characterized by a lead shock in the solid phase followed by a compaction layer which precedes the main reaction zone. In contrast, the reaction-led detonation on the right is characterized by a lead shock in the gas phase which is followed immediately by the main zone of reaction. Generally, reaction-led detonations are found for larger rates of compaction, larger rates of reaction and smaller rates of drag, while the converse is true of compaction-led detonations.

Evolution to detonation is found to consist of two stages in general. The first stage involves a relatively low speed compaction wave that propagates away from the piston face into the ambient explosive. Compaction is accompanied by a local rise in the temperature and pressure of both the phases. For the present model the pressure rise in the gas triggers reaction in the compacted region. The reaction generates gaseous product which, being unable to permeate into the compacted solid beyond a shallow depth, suffers a rise in pressure due to confinement. The higher gas pressure strengthens the reaction, resulting in more rapid gas production and hence still further gas pressurization. The process self-reinforces, and the amplifying pressure pulse steepens into a shock in the gas phase. Within the reaction zone behind the shock there is velocity disequilibrium between the phases, and the drag resulting therefrom transfers stress from the gas to the solid. The nozzling effect is an additional and significant source of stress transfer at this early stage, and the result is a compression of the solid in the reaction zone. This compression is transmitted acoustically to the solid upstream of the gas shock where the gas pressure is low, and the resulting pressure difference between the phases raises the local level of compaction. Eventually, the compressive disturbance in the solid
Figure 1: Representative profiles of the solid volume fraction $\bar{\alpha}$ for steady two-phase detonation structures: (a) compaction-led detonation and (b) reaction-led detonation. Symbols denote granular explosive $E$, compaction layer $C$, main reaction zone $R$, reaction products $P$, solid-phase shock $\bar{S}$, gas-phase shock $S$ and detonation velocity $D$.

steepens into a shock as well, thereby signalling the transition to a high-speed wave and the beginning of the second stage of evolution. Depending on the parameters of the model, the shock in the solid phase may or may not be overtaken at a later time by the shock in the gas phase, and this ultimately selects whether the long-time steady detonation is reaction-led or compaction-led. In either case, the steady detonation velocity obtained in our numerical calculations is close to, but slightly larger than, the theoretically determined Chapman-Jouguet (CJ) velocity, and the state of the gas at the end of the reaction zone where the solid phase has vanished lies on the weak branch of the fully-reacted Hugoniot.

An important element of the present work is the development of a numerical method for accurate solution of the hyperbolic system of partial differential equations governing the two-phase model. This system poses a numerical challenge due to its nonlinearity and stiffness of the source terms. As already observed, the nozzling terms involving derivatives of the solid volume fraction add to the difficulty because they cannot be cast in conservation form and thus standard numerical shock-capturing schemes based on discrete conservation do not apply. Previous numerical approaches have avoided this difficulty by omitting the nozzling terms altogether [5, 6], while others have discretized the nozzling terms based on the property that flows with uniform pressure and velocity, the so-called free-streaming flows, should be preserved in the time-stepping procedure [7, 8]. The numerical method used here follows a different approach which builds on previous work by the present authors [14]. In that paper the Riemann problem and an associated Godunov method are considered for the present two-phase model but without the undifferentiated source terms. For the Riemann problem the effect of the nozzling terms is confined to the contact discontinuity of the solid phase. Following the approach in [14] we treat the discontinuity as a layer of vanishing thickness within which the solution is smooth. This enables us to obtain jump conditions that connect the state of the solution on either side of the layer and provide a prescription for the numerical treatment of the nozzling terms. The treatment in the earlier paper considered an ideal equation of state for the gas phase whereas a virial equation of state is used here. This change requires only small modifications to the numerical approach. The Godunov method is extended to second-order accuracy following the approach in [14], and this becomes one step in a Strang-type fractional-step scheme. The other step is new, involves a numerical integration of the stiff source terms, and is handled by a Runge-Kutta error-control scheme similar to that employed in [15]. Finally, the grid resolution is increased locally near shocks and contacts, and in regions of rapid reaction and relaxation, using a scheme of adaptive mesh refinement (AMR). This enables us to compute highly-refined and accurate solutions with numerical efficiency.

Recent papers have considered reduced two-phase models in which velocity and/or pressure are equilibrated between the phases (see [10, 11, 12] for example). These models, which have fewer unknowns in the governing equations, may be considered to be approximations of the BN model. Indeed, the governing
equations in [10, 11] were derived as asymptotic reductions of the full BN model in the limits of very large drag and very rapid compaction. However the asymptotic analysis, originally carried out in a chemically inert context, retains validity in the presence of reaction only if the reaction rate is much slower than both the rate of compaction and the rate of drag-driven exchange of momentum between the phases. The aforementioned ability to compute well-resolved numerical solutions of the full BN model for a wide range of parameters, including large drag and rapid compaction, allows us to examine the accuracy of the asymptotic reductions in the presence of reaction whether the rate is small or large. For the case of very large drag, we find compaction-led detonations with thin layers of velocity disequilibrium but relatively wide layers of pressure disequilibrium. On the other hand, for the case of very rapid compaction, we find reaction-led detonations in which pressure is nearly equilibrated but with relatively wide layers in which the velocity is not. So the two limiting cases appear to compete. Furthermore, detonation structures in the full model typically exhibit separated shocks in the two phases, whereas reduced models with velocity and pressure equilibration necessarily involve single shocks. These findings cast doubt on the reduced models as accurate approximations of the full BN model for detonation evolution and structure.

The remainder of the paper is organized as follows. In Section 2, the governing equations of the full model are presented. This is followed in Section 3 with a discussion of the equations for traveling wave detonations. An analysis of the end state of a steady detonation is carried out in Section 4. The data set and reference states for the model are given in Section 5 for a chosen ambient state of the explosive and for assumed equations of state of the two phases. The numerical method used to obtain well-resolved solutions of the governing equations is described in Section 6, and this is followed in Section 7 with a presentation of the numerical results. Conclusions drawn from our work are discussed in Section 8.

2 Mathematical Model

We consider a variant of the two-phase Baer-Nunziato (BN) model originally presented in [1]. The model describes the behavior of granular explosives in which a gas occupies the pores between chemically reactive solid grains. It is assumed that each phase is a continuum and that the phases coexist at any point in space and time. The model consists of balance laws for mass, momentum and energy for each phase together with a compaction law and a saturation constraint. For the purposes of this paper we consider flow in one space dimension. Only a brief description of the model is given here; a more detailed description can be found in the original paper [1], or in the more recent paper by Bdzil et al [9].

The flow at position $x'$ and time $t'$ is specified by the density $\rho'$, velocity $u'$, pressure $p'$, temperature $T'$, total energy $E'$ and volume fraction $\alpha$ of the gas phase, and by the corresponding quantities for the solid phase denoted with over-bars. Dimensional quantities are specified by attaching a prime to the corresponding symbols, while symbols without a prime denote dimensionless quantities. We introduce the reference quantities

$$
t_{\text{ref}}', \quad u_{\text{ref}}', \quad p_{\text{ref}}', \quad x_{\text{ref}} = u_{\text{ref}}' t_{\text{ref}}', \quad \rho_{\text{ref}} = \frac{p_{\text{ref}}'}{u_{\text{ref}}'^2}, \quad T_{\text{ref}} = \frac{u_{\text{ref}}'^2}{C_{v,\text{ref}}'}, \quad E'_{\text{ref}} = u_{\text{ref}}'^2, \tag{1}
$$

where $C_{v,\text{ref}}'$ is a reference specific heat at constant volume, and use these as reference scales to define dimensionless quantities for both phases. (A particular choice for these reference quantities is made later in
In terms of dimensionless quantities, the system of governing equations is

\[
\frac{\partial \tilde{\alpha}}{\partial t} = -\frac{\partial \tilde{\alpha}}{\partial \tilde{x}} + \mathcal{F} + \frac{\mathcal{C}}{\tilde{\rho}},
\]

(2)

\[
\frac{\partial}{\partial t} (\tilde{\alpha} \tilde{p}) + \frac{\partial}{\partial \tilde{x}} (\tilde{\alpha} \tilde{p} \tilde{u}) = \mathcal{C},
\]

(3)

\[
\frac{\partial}{\partial t} (\tilde{\alpha} \tilde{p} \tilde{u}) + \frac{\partial}{\partial \tilde{x}} (\tilde{\alpha} (\tilde{p} \tilde{u}^2 + \tilde{p})) = \tilde{p} \frac{\partial \tilde{\alpha}}{\partial \tilde{x}} + \mathcal{M},
\]

(4)

\[
\frac{\partial}{\partial t} (\tilde{\alpha} \tilde{p} \tilde{E}) + \frac{\partial}{\partial \tilde{x}} (\tilde{\alpha} (\tilde{p} \tilde{E} + \tilde{p})) = \tilde{u} \tilde{p} \frac{\partial \tilde{\alpha}}{\partial \tilde{x}} - \tilde{p} \mathcal{F} + \mathcal{E},
\]

(5)

\[
\frac{\partial}{\partial t} (\alpha \rho) + \frac{\partial}{\partial \tilde{x}} (\alpha \rho \tilde{u}) = -\mathcal{C},
\]

(6)

\[
\frac{\partial}{\partial t} (\alpha \rho \tilde{E}) + \frac{\partial}{\partial \tilde{x}} (\alpha (\rho \tilde{E} + \rho)) = -\tilde{p} \frac{\partial \tilde{\alpha}}{\partial \tilde{x}} - \mathcal{M},
\]

(7)

\[
\frac{\partial}{\partial \tilde{t}} (\alpha \rho^2) + \frac{\partial}{\partial \tilde{x}} (\alpha \rho (\rho^2 + \rho)) = -\tilde{u} \tilde{p} \frac{\partial \tilde{\alpha}}{\partial \tilde{x}} + \tilde{p} \mathcal{F} - \mathcal{E},
\]

(8)

with the saturation constraint \( \alpha + \tilde{\alpha} = 1 \). Equation (2) describes the compaction of the solid phase, while (3), (4) and (5) are balance laws of mass, momentum and energy, respectively, for the solid. Mass, momentum and energy balances for the gas phase are specified by (6), (7) and (8), respectively.

The total energies in (5) and (8) are given by

\[
\tilde{E} = \bar{e}_{\text{ref}} + \frac{\dot{u}^2}{2}, \quad E = e + \frac{u^2}{2},
\]

where \( e \) is the specific internal energy of the gas and \( \bar{e}_{\text{ref}} = \bar{e} + B(\bar{\alpha}) \) is the specific internal energy of the solid, both made dimensionless using \( E_{\text{ref}}' = u_{\text{ref}}'^2 \). The internal energy of the solid is the sum of the internal energy of the pure solid \( \bar{e} \) and the compaction potential energy \( B(\bar{\alpha}) \). The compaction potential accounts for the configuration-dependent energy of the solid (see [9]). We employ a stiffened equation of state for the solid phase,

\[
\bar{e}(\bar{\rho}, \bar{\rho}) = \frac{\bar{p} + \bar{\pi}}{(\bar{\gamma} - 1)\bar{\rho}} + q,
\]

(9)

where \( \bar{\gamma} \) is the ratio of specific heats for the solid, \( \bar{\pi} = \bar{\pi}'/\rho_{\text{ref}}' \) is a dimensionless stiffening pressure, and \( q = q'/E_{\text{ref}}' \) is the dimensionless heat release. The gas phase is modeled by a virial equation of state,

\[
e(\rho, p) = \frac{p}{(\gamma - 1)\rho(1 + b \rho)},
\]

(10)

where \( b = b' \rho_{\text{ref}}' \) is a data-fit parameter (see Section 5). The corresponding sound speeds and temperatures of the phases are given by

\[
\tilde{c}^2 = \frac{\bar{\gamma}(\bar{p} + \bar{\pi})}{\bar{\rho}}, \quad c^2 = \frac{\gamma p}{\rho} \left[ 1 + b \rho - \frac{b^2 \rho^2}{\gamma(1 + b \rho)} \right],
\]

(11)

and

\[
\tilde{C}_vT = \frac{\bar{p} + \bar{\pi}}{(\bar{\gamma} - 1)\bar{\rho}}, \quad C_vT = \frac{p}{(\gamma - 1)\rho(1 + b \rho)},
\]

respectively, where the dimensionless specific heats at constant volume are given by \( \tilde{C}_v = \bar{C}_v'/\bar{C}_{v,\text{ref}}' \) and \( C_v = C_v'/C_{v,\text{ref}}' \).

Many choices can be made for the equations of state for the solid and gas phases. The simplest choice is an ideal equation of state for both phases, but this choice does not provide enough flexibility to match sound speeds and detonation speeds for typical condensed-phase explosives. The choices given in (9) and (10) are minor extensions of an ideal equation of state. These have been used by others (see [9] and [16] for example) for being relatively simple and yet general enough to match physical speeds characteristic of typical explosives. More elaborate equations of state for specific explosives have also been employed. For example, a JWL equation of state for the gas phase of the explosive CP was used in [17].
The source terms on the right-hand-sides of the governing equations involve non-conservative differentiated source terms and undifferentiated exchange terms. The non-conservative, or nozzling, terms are proportional to the gradient of the volume fraction, \( \partial \alpha / \partial x \). These terms model interphase momentum and energy transfer that occurs as a result of an effective change in the cross-sectional area of the virtual stream tube of the gas phase. The exchange source terms include the conversion of energetic solid to gaseous products due to chemical reaction, and the exchange of mass, momentum and energy due to the relaxation processes of compaction, drag and heat transfer.

The exchange of mass between phases is due to chemical reaction which is specified by \( C \). We assume that the reaction converts solid grains of the explosive into gaseous products in which case \( C < 0 \). The precise expression for \( C \) depends on the particulars of the chemical kinetics. For the purposes of this paper, we employ a simple reaction rate model of the form

\[
C = \begin{cases} 
-\sigma \tilde{\alpha} \tilde{\rho}(\bar{p} - p_{\text{ign}}), & \text{if } p > p_{\text{ign}}, \\
0, & \text{otherwise}, 
\end{cases} 
\]

where \( \sigma = \sigma' t_{\text{ref}}' \) is a reaction rate prefactor and \( p_{\text{ign}} = p'_{\text{ign}} / p_{\text{ref}}' \) is an ignition pressure. For this pressure-dependent model, the reaction is off when the gas pressure is less than \( p_{\text{ign}} \), and increases linearly with \( p \) when \( p > p_{\text{ign}} \). The choice made here is similar to that used in [1].

The source term for the compaction law in (2) involves the reaction rate defined in (12) and the compaction rate \( \mathcal{F} \), which is taken to be

\[
\mathcal{F} = \tilde{\alpha} \alpha \tilde{\rho} (\bar{p} - \beta),
\]

where \( \mu_c = \mu_c' / (p_{\text{ref}}' t_{\text{ref}}') \) is the compaction viscosity and \( \beta = \beta' / p_{\text{ref}}' \) is the configuration pressure. Since \( C < 0 \), the reaction rate tends to de-compact the mixture, while \( \mathcal{F} \) may compact or de-compact the mixture depending on the sign of \( \bar{p} - \beta \). In the absence of chemical reaction (i.e. if \( C = 0 \)), the compaction rate provides a relaxation mechanism which drives the mixture towards pressure equilibrium, \( \bar{p} = p + \beta \), with the compaction viscosity \( \mu_c \) characterizing the compaction rate. The solid grains are subjected to pressure exerted by the gas, as well as by inter-granular forces. Thus, at equilibrium the phase pressures are offset by \( \beta \), which represents the grain-to-grain contact stresses [1, 9]. The configuration pressure is related to the compaction potential energy through the relation

\[
\beta(\tilde{\alpha}, \tilde{\rho}) = \tilde{\alpha} \tilde{\rho} dB(\tilde{\alpha}).
\]

Following the choice made in [16], we take

\[
\beta = -(p_0 - \tilde{p}_0) \tilde{\alpha} \tilde{\rho} \left( \frac{2 - \alpha_0}{2 - \tilde{\alpha}} \right) \frac{\ln (1 - \tilde{\alpha})}{\ln (1 - \alpha_0)},
\]

where the zero subscript denotes quantities in a quiescent uniform mixture. Integration with respect to \( \tilde{\alpha} \), subject to the condition \( B(\tilde{\alpha}_0) = 0 \), determines \( B(\tilde{\alpha}) \) to be

\[
B(\tilde{\alpha}) = \frac{(p_0 - \tilde{p}_0)(2 - \alpha_0)^2 \tilde{\alpha}}{\alpha_0 \tilde{\rho}_0 \ln (1 - \alpha_0)} \ln \left( \frac{2 - \alpha_0}{2 - \tilde{\alpha}} \right) \frac{(1 - \tilde{\alpha})(1 - \alpha_0)/(2 - \tilde{\alpha})}{(1 - \alpha_0)(1 - \alpha_0)/(2 - \alpha_0)}. \]

(We note that there is an error in the formula for \( B(\tilde{\alpha}) \) given in [16].)

The residual momentum exchange \( \mathcal{M} \), which appears on the right-hand-side of (4) and (7), is associated with burning and drag and is taken to be

\[
\mathcal{M} = C \bar{u} + \left( \frac{\delta + \frac{1}{2} C}{\tilde{\rho}} \right) (u - \bar{u}).
\]

The drag term provides a relaxation mechanism which drives the phases toward velocity equilibrium, \( \bar{u} = u \), with the interphase drag coefficient \( \delta = \delta t_{\text{ref}}' / p_{\text{ref}}' \) characterizing the rate. The residual energy exchange \( \mathcal{E} \) due to burning, drag, and interphase heat transfer appears in (5) and (8), and is given by

\[
\mathcal{E} = \left( \frac{\delta + \beta}{\tilde{\rho}} \right) C + \left( \mathcal{M} - C \bar{u} \right) \bar{u} + \mathcal{H}(T - \bar{T}),
\]
where \( \mathcal{H} = \mathcal{H}'_{\text{ref}}/(\rho'_{\text{ref}} C_{v,\text{ref}}') \) is the interphase heat transfer coefficient.

Though mass, momentum, and energy are not conserved for the phases individually, these quantities are conserved for the mixture. The mass, momentum, and energy equations of the two phases may be combined to yield conservation equations for the mixture,

\[
\begin{align*}
\frac{\partial}{\partial t} (\bar{\rho} + \alpha \rho) + \frac{\partial}{\partial x} (\bar{\rho} \bar{u} + \alpha \rho u) &= 0, \quad (15) \\
\frac{\partial}{\partial t} (\bar{\rho} \bar{u} + \alpha \rho u) + \frac{\partial}{\partial x} (\bar{\rho} \bar{u}^2 + \bar{p}) + \alpha (\rho u^2 + p) &= 0, \quad (16) \\
\frac{\partial}{\partial t} (\bar{\rho} E + \alpha \rho E) + \frac{\partial}{\partial x} (\bar{\rho} \bar{u} (\bar{E} + \bar{p}) + \alpha u (E + p)) &= 0. \quad (17)
\end{align*}
\]

These equations are used to obtain algebraic constraints for steady traveling wave solutions as noted below.

### 3 Steady Traveling Detonations

In this section we consider the equations for steady detonation waves. These equations are obtained from the governing system (2)–(8), and involve ordinary differential equations (ODEs) in terms of the variable \( \xi = x - Dt \), where \( D \) is the constant detonation velocity. The ODEs hold for smooth portions of the detonation structure, and are supplemented by Rankine-Hugoniot jump conditions which hold across shocks in either of the phases. The derivation of the equations and their analysis is similar to that for a single-phase reactive flow. Details are not given here, but can be found in [4] for the two-phase model of Powers, Stewart and Krier. Suffice it to say that the structure problem can be reduced to a differential-algebraic system of four ODEs and three algebraic equations, the latter being the expressions of conservation of mass, momentum and energy of the two-phase mixture.

The system of ODEs possesses singularities at points in the flow where the particle velocity relative to the wave for either phase is zero or sonic, and where either \( \alpha = 0 \) or \( \bar{\alpha} = 0 \). Our numerical experiments (Section 7) show that \( \alpha = 0 \) is not reached, but that \( \bar{\alpha} = 0 \) is attained at the end of the detonation structure where the solid reactant vanishes. Also, we find that the velocities of the phases relative to the steady wave do not vanish (as in the single-phase case), but that the relative velocity of the gas phase may accelerate smoothly through sonic in the interior of the detonation structure. For such a case, an additional constraint on the flow is needed to remove the singularity. Ultimately, traveling wave solutions, including the value for \( D \), would need to be constructed by patching regions of smooth flow where the ODEs apply together with jump conditions across shocks (which may lead the wave or be an internal jump), removable-singularity constraints, and of course suitable boundary conditions. The main difficulty in constructing such solutions is that the precise structure is not known ahead of time. Therefore we do not pursue the ODE approach here but rather, obtain steady solutions numerically though time integration of the unsteady system. We recognize that this computational approach will only find those steady traveling-wave solutions that are stable. Whether the present model admits unstable, steady traveling waves remains an open question. Asymptotically unsteady solutions are, of course, accessible using our computational approach, but none were found for the parameter range under study.

It is useful to follow the state of the mixture through the wave. The analysis here is similar to that given in [18]. From (15)–(17) and their corresponding integral conservation laws, we have

\[
\begin{align*}
\bar{\alpha} \bar{\rho} \bar{w} + \alpha \rho w &= Q_0, \quad (18) \\
\bar{\alpha} \bar{w} (\bar{p} + \bar{w}^2) + \alpha (p \bar{w}^2 + \bar{p}) &= P_0, \quad (19) \\
\bar{\alpha} \bar{\rho} \bar{w} \left( \bar{e} + B(\bar{\alpha}) + \frac{\bar{w}^2}{2} + \frac{\bar{p}}{\bar{\rho}} \right) + \alpha \rho w \left( e + \frac{w^2}{2} + \frac{p}{\rho} \right) &= S_0, \quad (20)
\end{align*}
\]

where \( \bar{w} = \bar{u} - D \) and \( w = u - D \) are flow velocities in the detonation-fixed frame and \( Q_0 \), \( P_0 \), and \( S_0 \)
are constants. These equations suggest the mixture quantities
\[
\rho_m = \bar{\alpha} \bar{\rho} + \alpha \rho, \quad (21)
\]
\[
\rho_m u_m = \bar{\alpha} \bar{\rho} \bar{u} + \alpha \rho \bar{u}, \quad (22)
\]
\[
p_m = \bar{\alpha} \bar{\rho} + \alpha \rho + \frac{(u - \bar{u})^2}{1/(\bar{\alpha} \bar{\rho}) + 1/(\alpha \rho)}, \quad (23)
\]
\[
\rho_m e_m = \bar{\alpha} \bar{\rho} \bar{e} + \alpha \rho e. \quad (24)
\]

Other choices for mixture variables can be made (see [16] and [18], for example) but the ones given here are suitable for the purposes of the present analysis. Assuming that the mixture is at rest in the uniform state upstream of the detonation (i.e. \( \bar{u}_0 = u_0 = 0 \)), we have
\[
Q_0 = -\rho_{m0} D, \quad (27)
\]
\[
P_0 = -Q_0 D + p_{m0}, \quad (28)
\]
\[
S_0 = \frac{1}{2} Q_0 D^2 - (e_{m0} + P_0) D, \quad (29)
\]
where the upstream mixture quantities are given by
\[
\rho_{m0} = \bar{\alpha}_0 \bar{\rho}_0 + \alpha_0 \rho_0, \quad (25)
\]
\[
p_{m0} = \bar{\alpha}_0 \bar{p}_0 + \alpha_0 p_0, \quad (30)
\]
\[
\rho_{m0} e_{m0} = \bar{\alpha}_0 \bar{\rho}_0 \bar{e}_0 + \alpha_0 \rho_0 e_0. \quad (31)
\]

In terms of the mixture quantities \( \rho_m, u_m \) and \( p_m \) defined in (21), (22) and (23), respectively, (18) and (19) take the form
\[
\rho_m (u_m - D) = -\rho_{m0} D, \quad (27)
\]
\[
\rho_m u_m (u_m - D) + p_m = p_{m0}. \quad (28)
\]
We may eliminate \( D \) from these two equations to find
\[
u_m^2 = (p_m - p_{m0}) (v_{m0} - v_m), \quad v_m = 1/\rho_m, \quad v_{m0} = 1/\rho_{m0}, \quad (25)
\]
or we may eliminate \( u_m \) to obtain
\[
p_m = p_{m0} - \rho_{m0}^2 D^2 (v_m - v_{m0}). \quad (26)
\]
The latter equation involving the pressure and specific volume of the mixture is analogous to the Rayleigh line relation obtained for single-phase flow with \( D \) specifying the slope of the line in the \( p_m - v_m \) plane.

Following the usual analysis for single-phase flow, the next step would be to derive a family of Hugoniot curves for \( p_m \) as a function of \( v_m \), parameterized by \( \bar{\alpha} \), say, from the conservation constraints in (18), (19) and (20). Such a derivation does not appear to be possible for the two-phase equations. However, the fully-reacted Hugoniot curve corresponding to \( \bar{\alpha} = 0 \) can be found because then the mixture consists of the gas phase only. The intersection of this Hugoniot and the mixture Rayleigh line in (26) determines possible end states of the steady detonation wave and defines a Chapman-Jouguet (CJ) state as we discuss in the next section.

4 End-State Analysis

The end state of the steady system corresponds to a complete conversion of the solid grains, and thus consists of only gaseous particles. At the end state, where \( \bar{\alpha} = 0 \), the mixture density, velocity, pressure and energy defined in (21), (22), (23), and (24), respectively, reduce to those of the gas phase, and the conservation constraints in (18), (19) and (20) become
\[
\rho_f (u_f - D) = Q_0, \quad (27)
\]
\[
\rho_f (u_f - D)^2 + p_f = P_0, \quad (28)
\]
\[
\rho_f (u_f - D) \left( e_f + \frac{(u_f - D)^2}{2} + \frac{p_f}{\rho_f} \right) = S_0, \quad (29)
\]
where the subscript \( f \) denotes end-state gas variables. The first two constraints may be used to obtain
\[
 u_f^2 = (p_f - p_m)(v_m - v_f), \quad p_f = p_m - \rho_f^2 D^2 (v_f - v_m), \quad v_f = 1/\rho_f, \quad (30)
\]
which correspond to (25) and (26) evaluated at the end state, and all three constraints along with (10) may be used to obtain a fully-reacted Hugoniot which has the form
\[
p_f = \frac{\mu(v_f + b) [2e_m - p_m (v_f - v_m)]}{v_f^2 - \mu(v_m - b)v_f - \mu(bv_m)}, \quad \mu = \frac{\gamma - 1}{\gamma + 1}, \quad (31)
\]
Figure 2 shows the construction of the steady solution in the \( p_m - v_m \) plane. The fully-reacted Hugoniot curve given by (31) has two vertical asymptotes, one for \( v_f < 0 \) and one for \( v_f > 0 \). The only physically admissible branch of the curve is the one which lies to the right of both asymptotes, and this is the one shown in the figure. The Rayleigh line, shown for three values of \( D \), is given by (26). For a given value of \( D \), the Rayleigh line intersects the fully-reacted Hugoniot at two points, one point or not at all. The borderline case occurs when the Rayleigh line is tangent to the Hugoniot, and the slope of this line determines the CJ detonation velocity, \( D_{CJ} \), which is the minimum allowable velocity for a steady solution. For \( D < D_{CJ} \), there are no intersections and no steady solutions, and for \( D > D_{CJ} \) there are steady solutions corresponding to two detonation speeds, one on the so-called strong branch with \( p_f > p_{CJ} \) and the other on the weak branch with \( p_f < p_{CJ} \) (see [19]). The end state of the steady detonations found later (see Figure 17) lies on the weak branch of the fully-reacted Hugoniot near the CJ point.

A formula for \( D_{CJ} \) may be found by equating the slope of the fully-reacted Hugoniot with the slope of the Rayleigh line at \( v_{CJ} \). This condition gives
\[
 D_{CJ}^2 = \frac{\mu v_{m0}^2 \{ (1 - \mu) [p_{m0}(v_{m0} - b) v_{CJ}^2 + 2b p_m v_{m0} v_{CJ} - 2b^2 e_m] + 2 e_m (v_{CJ} + b)^2 \} }{[v_{CJ}^2 - \mu(v_m - b)v_{CJ} - \mu(bv_m)]^2}, \quad (32)
\]
where \( v_{CJ} \) is determined by the quartic
\[
 a_4 v_{CJ}^4 + a_3 v_{CJ}^3 + a_2 v_{CJ}^2 + a_1 v_{CJ} + a_0 = 0, \quad (33)
\]
which has coefficients given by

\[ a_0 = 2\mu^2 b^2 v_{m0} (2e_{m0} + p_{m0} v_{m0}), \]
\[ a_1 = 2\mu b [2e_{m0} ((1 + \mu) v_{m0} - \mu b) + p_{m0} v_{m0} ((1 + \mu) v_{m0} - 2\mu b)], \]
\[ a_2 = [2\mu e_{m0} ((1 + \mu) v_{m0} - (3 + \mu) b) + \mu p_{m0} ((1 + \mu) v_{m0}^2 - 2b(3 + \mu) v_{m0} + 2\mu b^2)], \]
\[ a_3 = -4\mu [e_{m0} + p_{m0} (v_{m0} - b)], \]
\[ a_4 = (1 + \mu)p_{m0}. \]

The roots of (33) may be found numerically using Newton’s method for example. Alternatively, an analytic solution may be found assuming that \( \frac{v_{m0}p_{m0}}{e_{m0}} \ll 1. \)

In this limit, one root of the quartic tends to infinity while the remaining three roots (including the root of interest) solve the cubic

\[ v_{CJ}^3 + A_2 v_{CJ}^2 + A_1 v_{CJ} + A_0 = 0, \]

where

\[ A_0 = -\mu b^2 v_{m0}, \]
\[ A_1 = -b [(1 + \mu) v_{m0} - \mu b], \]
\[ A_2 = -\frac{1}{2} [(1 + \mu) v_{m0} - (3 + \mu) b]. \]

We note that for the upstream state given later in Table 2, we have

\[ \frac{v_{m0}p_{m0}}{e_{m0}} = 4.55 \times 10^{-4}, \]

so that the approximation is reasonable. Accepting this approximation, the three roots of (34) can be found explicitly. In particular, the root on the appropriate branch of the fully-reacted Hugoniot corresponding to the CJ point is given by

\[ v_{CJ} = \frac{1}{3} \left( \chi \cos \vartheta - A_2 \right), \]

where

\[ \chi = (1 + \mu) v_{m0} + (3 - \mu) b, \quad \vartheta = \frac{1}{3} \cos^{-1} \left[ \frac{4}{\chi^3} (9A_1 A_2 - 27A_0 - 2A_2^2) \right]. \]

The CJ detonation velocity is now determined by (32) with \( v_{CJ} \) given by (35), and the corresponding flow velocity and pressure at the CJ state are given by (30) with \( v_f = v_{CJ}. \)

Now that the possible end states have been established, and in particular the CJ state, we consider the behavior of the steady solution as the end state is approached. A simple analysis of the structure problem shows that the approach to \( \bar{\alpha} = 0 \) is exponential and occurs in the limit \( \xi \to -\infty. \) This behavior is analogous to that for single-phase reactive flow for a reaction rate with linear depletion. Further, it is found that the phase velocities and temperatures equilibrate as the end state is approached, but that the phase pressures need not equilibrate. This last assertion is a consequence of the fact that according to (13), vanishing of \( \bar{\alpha} \) at the end state is enough to ensure the vanishing of the compaction rate \( F \) there.

5 Data Set and Reference States

In the numerical results presented later in Section 7, we study the evolution to detonation and the behavior of the steady detonation structure for a range of parameters involving the reaction rate and relaxation processes. For these numerical experiments we consider a representative explosive with upstream state given by

\[ \bar{\alpha}_0 = .73, \quad \alpha_0 = .27, \]
\[ \bar{\rho}_0' = 1900 \text{ kg/m}^3, \quad \rho_0' = 1 \text{ kg/m}^3, \]
\[ \bar{p}_0 = 7.6 \text{ MPa}, \quad p_0' = .25225 \text{ MPa}, \]

\[ \text{where } \bar{\alpha}_0 = \frac{\alpha_0}{\rho_0' / \rho_0}, \text{ and } \bar{\rho}_0' = \frac{\rho_0'}{\rho_0}, \]
and with equation of state parameters given by
\[ \bar{\gamma} = 5, \quad \gamma = 1.35, \]
\[ \bar{\pi}' = 3412.4 \text{ MPa}, \quad b' = 0.001 \text{ m}^3/\text{kg}, \]
\[ \bar{C}'_v = 1500 \text{ J/(kg K)}, \quad C'_v = 2400 \text{ J/(kg K)}. \]

The heat release is taken to be \( q' = 6.65 \times 10^6 \text{ J/kg}, \)
which is a typical value for polymer-bonded explosives (PBXs). For this choice, the upstream temperatures and sound speeds are
\[ T'_0 = T'_0 = 300 \text{ K}, \quad \bar{c}'_0 = 3000 \text{ m/s}, \quad c'_0 = 583.85 \text{ m/s}. \]

The value of \( b' \) in the virial equation of state for the gas phase has a strong effect on the CJ state, and in particular the detonation velocity \( D'_{CJ} \). Figure 3 shows the behavior of \( D'_{CJ} \) versus \( b' \) for the upstream state given above. (A similar plot is reported in [18].) For \( b' = 0.001 \text{ m}^3/\text{kg} \), we find
\[ D'_{CJ} = 7508.8 \text{ m/s}, \]
which is in the range of most PBXs. For this choice, the density, velocity and pressure at the CJ state are found to be
\[ \rho'_{CJ} = 1/\bar{\rho}'_{CJ} = 1906.2 \text{ kg/m}^3, \quad u'_{CJ} = 2044.3 \text{ m/s}, \quad p'_{CJ} = 21.300 \text{ GPa}. \]

From these values, we compute the corresponding temperature and sound speed to be
\[ T'_{CJ} = 4577.1 \text{ K}, \quad c'_{CJ} = 5464.5 \text{ m/s}. \]

It is noted that for an ideal equation of state in which \( b' = 0 \), the CJ detonation velocity is less than 4000 m/s, an unrealistically low value for typical condensed-phase explosives.

Reference scales may be defined, following (1), using the CJ detonation speed and pressure, and the choice \( t'_{\text{ref}} = 1 \mu s \) and \( C'_{v,\text{ref}} = C'_v \). These scales are collected in Table 1. With reference scales in hand, we may now compute the dimensionless upstream state and CJ state, which is given in Table 2. Dimensionless equation of state parameters may be computed as well, and these are provided in Table 3.

The remaining parameters of the two-phase model involve the reaction rate and relaxation source terms. Choices for these parameters are discussed later in Section 7 in the context of our study of the detonation.
structure as these parameters vary. For reference, we provide a list of the choices for the relaxation parameters \( \delta' \), \( \mu'_c \) and \( \mathcal{H}' \) made by others in Table 4. Using the reference scales

\[
\delta'_{\text{ref}} = \frac{\rho'_{\text{ref}}}{t'_{\text{ref}}}, \quad \mu'_{c,\text{ref}} = \frac{\mu'_{c,\text{ref}}}{t'_{\text{ref}}}, \quad \mathcal{H}'_{\text{ref}} = \frac{\rho'_{\text{ref}} C'_{v,\text{ref}}}{t'_{\text{ref}}},
\]

we also list the corresponding dimensionless parameters. Many of the entries in the table are taken directly from the reference cited, but some are estimated based on the available information given in the reference and our numerical results since the corresponding form for the source term is not the same as the one used here. For example, Baer and Nunziato [1] use an Ergun form for the drag coefficient, i.e.

\[
\delta' = \frac{\mu'_g}{\kappa_g} \left( 1 + \frac{\zeta_1 \text{Re}}{\alpha} \right),
\]

where \( \mu'_g = 5 \times 10^{-5} \text{ kg/(m s)} \) is the gas viscosity, \( \kappa_g = \alpha^{4.5} (d'_0)^2 / \zeta_2 \) is a permeability, \( \text{Re} = \alpha \rho' d'_0 |u' - \bar{u}'| / \mu'_g \) is a Reynolds number, \( d'_0 = 10^{-4} \text{ m} \) is the average initial grain diameter, and \( \zeta_1 = 0.01 \) and \( \zeta_2 = 33 \) are data-fit parameters. To estimate \( \delta' \) we use \( \alpha = \bar{\alpha} = 0.5, \rho' = 10^3 \text{ kg/m}^3 \) and \( |u' - \bar{u}'| = 10^4 \text{ m/s} \) which are nominal values for a velocity-disequilibrium layer in a steady detonation structure according to our numerical calculations. This leads to the value given in the table which works out to be much larger than the value used by the other references cited. It is important to keep in mind that the parameter values listed, whether obtained directly in a reference or estimated here, are all modeling choices. We use these as a guide, but consider the behavior of solutions for a wide range of the parameters.

### Table 1: Reference scales.

<table>
<thead>
<tr>
<th>Reference Scale</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t'_{\text{ref}} )</td>
<td>1</td>
<td>( \mu s )</td>
</tr>
<tr>
<td>( u'_{\text{ref}} )</td>
<td>7508.8</td>
<td>m/s</td>
</tr>
<tr>
<td>( p'_{\text{ref}} )</td>
<td>21.300</td>
<td>GPa</td>
</tr>
<tr>
<td>( C'_{v,\text{ref}} )</td>
<td>2400</td>
<td>J/(kg K)</td>
</tr>
<tr>
<td>( x'_{\text{ref}} )</td>
<td>7.5088</td>
<td>mm</td>
</tr>
<tr>
<td>( \rho'_{\text{ref}} )</td>
<td>377.78</td>
<td>kg/m(^3)</td>
</tr>
<tr>
<td>( T'_{\text{ref}} )</td>
<td>23492</td>
<td>K</td>
</tr>
<tr>
<td>( E'_{\text{ref}} )</td>
<td>( 5.6381 \times 10^4 )</td>
<td>J/kg</td>
</tr>
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</table>

### Table 2: Dimensionless upstream and CJ states.

<table>
<thead>
<tr>
<th>Solid EOS</th>
<th>Value</th>
<th>Gas EOS</th>
<th>Value</th>
<th>Solid EOS</th>
<th>Value</th>
<th>Gas EOS</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{\alpha} )</td>
<td>0.73</td>
<td>( \alpha_0 )</td>
<td>0.27</td>
<td>( \bar{D}_{\text{CJ}} )</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \bar{\rho}_0 )</td>
<td>5.0293</td>
<td>( \rho_0 )</td>
<td>2.6470 \times 10^{-5}</td>
<td>( \rho_{\text{CJ}} )</td>
<td>5.0459</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \bar{p}_0 )</td>
<td>( 3.5681 \times 10^{-4} )</td>
<td>( p_0 )</td>
<td>1.1843 \times 10^{-5}</td>
<td>( p_{\text{CJ}} )</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \bar{T}_0 )</td>
<td>0.012770</td>
<td>( T_0 )</td>
<td>0.012770</td>
<td>( T_{\text{CJ}} )</td>
<td>0.19483</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \bar{e}_0 )</td>
<td>0.39953</td>
<td>( e_0 )</td>
<td>0.077756</td>
<td>( u_{\text{CJ}} )</td>
<td>0.27225</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 3: Dimensionless equation of state parameters.

<table>
<thead>
<tr>
<th>Solid EOS</th>
<th>Value</th>
<th>Gas EOS</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{\gamma} )</td>
<td>5</td>
<td>( \gamma )</td>
<td>1.35</td>
</tr>
<tr>
<td>( \bar{c} )</td>
<td>0.16021</td>
<td>( c )</td>
<td>0.37778</td>
</tr>
<tr>
<td>( C'_{v,\text{ref}} )</td>
<td>0.625</td>
<td>( C_v )</td>
<td>1</td>
</tr>
<tr>
<td>( q )</td>
<td>0.11795</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Reference scales.
6 Numerical Method

In this section, we describe a numerical method for the time-dependent model equations in (2)–(8), which we rewrite in the form

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial f(\mathbf{u})}{\partial x} = h(\mathbf{u}) \frac{\partial \alpha}{\partial x} + k(\mathbf{u}),$$  \hspace{1cm} (36)

where

$$\mathbf{u} = \begin{bmatrix} \bar{\alpha} \\ \bar{\alpha} \bar{\rho} \\ \bar{\alpha} \bar{\rho} \bar{u} \\ \bar{\alpha} \bar{\rho} \bar{E} \\ \alpha \rho \\ \alpha \rho u \\ \alpha \rho E \end{bmatrix}, \quad f(\mathbf{u}) = \begin{bmatrix} 0 \\ \bar{\alpha} \bar{\rho} \bar{u} \\ \bar{\alpha} (\bar{\rho} \bar{u}^2 + \bar{p}) \\ \bar{\alpha} (\bar{\rho} \bar{E} + \bar{p}) \\ \alpha \rho u \\ \alpha (\rho u^2 + p) \\ \alpha u (\rho E + p) \end{bmatrix}, \quad h(\mathbf{u}) = \begin{bmatrix} -\bar{u} \\ 0 \\ \bar{p} \\ 0 \\ -p \\ 0 \end{bmatrix}, \quad k(\mathbf{u}) = \begin{bmatrix} F + C/\bar{\rho} \\ -C \\ +M \\ -C \\ -M \end{bmatrix}.$$

The method employs a second-order, Strang-type, fractional-step method of the form

$$\mathbf{U}_j^{n+1} = S_h(\Delta t/2) S_h(\Delta t) S_h(\Delta t/2) \mathbf{U}_j^n$$

where \( \mathbf{U}_j^n \) denotes the cell average of \( \mathbf{u}(x,t) \) on a grid \( x_j = j \Delta x \) at a time \( t_n \), and \( \Delta t \) is the time step from \( t_n \) to \( t_{n+1} \). The operators \( S_h(\tau) \) and \( S_h(\tau) \) represent numerical integrations of the equations

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial f(\mathbf{u})}{\partial x} = h(\mathbf{u}) \frac{\partial \alpha}{\partial x},$$  \hspace{1cm} (37)

and

$$\frac{\partial \mathbf{u}}{\partial t} = k(\mathbf{u}),$$  \hspace{1cm} (38)

respectively, over a time interval \( \tau \). The integration of (37) uses a second-order, slope-limited Godunov method, which is modified to handle the non-conservative nozzling terms following the approach described by the present authors in [14]. The integration of (38) uses a second-order, adaptive Runge-Kutta method similar to the one described by Henshaw and Schwendeman in [15] for the reactive Euler equations. Since the basic elements of the fractional-step method are described elsewhere, we focus here on the various modifications needed to handle the particular model equations at hand.

6.1 Godunov step and Riemann problem

The Godunov step, \( \tilde{\mathbf{U}}_j = S_h(\Delta t) \mathbf{U}_j \), uses a finite-volume discretization of the form

$$\tilde{\mathbf{U}}_j = \mathbf{U}_j - \frac{\Delta t}{\Delta x} \left( F_L(\mathbf{U}_{j,+}, \mathbf{U}_{j+1,-}) - F_R(\mathbf{U}_{j-1,+}, \mathbf{U}_{j,-}) \right) + \frac{\Delta t}{\Delta x} \tilde{H}_j,$$  \hspace{1cm} (39)

where \( F_s(\mathbf{U}_L, \mathbf{U}_R), \ s = L, R, \) are numerical flux functions depending on left and right states, \( \mathbf{U}_L \) and \( \mathbf{U}_R \), respectively, and \( \tilde{H}_j \) is a second-order correction to handle the non-conservative nozzling term. (The

<table>
<thead>
<tr>
<th>Reference</th>
<th>( \delta' )</th>
<th>( \mu'_c )</th>
<th>( \mathcal{H}' )</th>
<th>( \delta )</th>
<th>( \mu_c )</th>
<th>( \mathcal{H} )</th>
</tr>
</thead>
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<tr>
<td>[1]</td>
<td>( 7.5 \times 10^{10} )</td>
<td>( 2 \times 10^3 )</td>
<td>( 8 \times 10^8 )</td>
<td>200</td>
<td>.994</td>
<td>.0088</td>
</tr>
<tr>
<td>[6]</td>
<td>( 10^5 )</td>
<td>( 10^2 )</td>
<td>( 2.2 \times 10^3 )</td>
<td>.26</td>
<td>.0047</td>
<td>.00024</td>
</tr>
<tr>
<td>[11]</td>
<td>( 2 \times 10^8 )</td>
<td>( 2 \times 10^8 )</td>
<td>( 10^8 )</td>
<td>.53</td>
<td>.094</td>
<td>.011</td>
</tr>
<tr>
<td>[16]</td>
<td>( 10^5 )</td>
<td>( 10^7 )</td>
<td>( 10^{10} )</td>
<td>.26</td>
<td>.047</td>
<td>.11</td>
</tr>
</tbody>
</table>

Table 4: Relaxation parameters found in the literature. The units for \( \delta' \), \( \mu'_c \) and \( \mathcal{H}' \) are kg/(m^3)s, Pas and J/(K m^3)s, respectively.
superscript \( n \) is suppressed here for notational convenience.) The states \( \mathbf{U}_{j,\pm} \), are obtained using first-order, slope-limited Taylor approximations to the cell interface on the left (minus subscript) and the right (plus subscript) of the cell centered at \( x_j \). The numerical flux functions are based on solutions of Riemann problems for (37) centered at each cell interface using left and right states provided by the Taylor approximations, and they include (first-order) contributions from the nozzling terms. The full details of (39) are provided in [14] for the case of a stiffened equation of state for the solid phase and an ideal equation of state for the gas phase. For reasons discussed earlier, a virial equation of state is used here for the gas phase. Accordingly, the main modification of the Godunov step involves the solution of the Riemann problem for the case of a virial equation of state for the gas.

The solution of the Riemann problem for (37) with initial data \( \mathbf{u}(x,0) = \mathbf{U}_L \) for \( x < 0 \) and \( \mathbf{u}(x,0) = \mathbf{U}_R \) for \( x > 0 \) consists of constant states in each phase separated by transitions across characteristic fields involving the eigenvalues

\[
\begin{align*}
\lambda_1 &= \bar{u} - \bar{c}, \\
\lambda_2 &= \lambda_3 = \bar{u}, \\
\lambda_4 &= \bar{u} + \bar{c}, \\
\lambda_5 &= u - c, \\
\lambda_6 &= u, \\
\lambda_7 &= u + c,
\end{align*}
\]

of the hyperbolic PDE. For the nonlinear acoustic fields, \( \bar{u} \pm \bar{c} \) and \( u \pm c \), the transitions are shocks or rarefactions across which \( \bar{\alpha} \) is constant so that the phases decouple. (Figure 4 gives a representative solution.) Formulas for these transitions follow from the usual analysis of the Euler equations for each phase separately. The linear fields, \( \bar{u} \) and \( u \), are contact discontinuities. The gas contact is benign and behaves as a usual contact discontinuity for the gas phase separately (assuming \( u \neq \bar{u} \)). The behavior of the solid contact, on the other hand, is more complex since it is here that the phases couple in the solution of the Riemann problem. A thin-layer analysis of the solid contact is discussed in [14], which provides jump conditions involving the mass, momentum, enthalpy, entropy and the solid velocity across the contact. For the case of a virial equation of state for the gas, we revisit the various formulas for the transitions across shocks and rarefactions for the gas, and the formulation of the jump conditions across the solid contact.

![Figure 4: A representative solution of the Riemann problem consisting of shocks, rarefactions and contact discontinuities indicated by the symbols \( S, R \) and \( C \), respectively.](image)

The analysis in [14] is restricted primarily to the case when the solid contact lies between the shocks and rarefactions of the gas, i.e. when

\[
(u - \bar{u})^2 < c^2,
\]

as shown in Figure 4. This case, sometimes referred to as the subsonic case, is relevant for flows involving high drag between phases, as is usually the case for granular explosives and as is considered here. We specifically exclude passage through the sonic singularity for which a unique solution of the corresponding Riemann problem is presently unavailable (see [20] and [21]).

The notation used to denote the intermediate states in the solution of the Riemann problem is indicated in Figure 5 for a representative solution configuration in which the solid contact lies to the left of the gas contact. We assume that quantities with subscript 1 lie to the right of the transitions in the \( \bar{u} - \bar{c} \) and \( u - c \) characteristic fields, while quantities with subscript 2 lie to the left of the transitions in the \( \bar{u} + \bar{c} \) and \( u + c \)
characteristic fields. For the case of an ideal or stiffened equation of state it is convenient to parameterize
the density and velocity of these intermediate states with pressure. Following [14], we define

$$ u_1 = \bar{u}_L - \bar{F}_L(\bar{p}_1), \quad \bar{p}_1 = \bar{G}_L(\bar{p}_1), \quad \bar{u}_2 = \bar{u}_R + \bar{F}_R(\bar{p}_2), \quad \bar{p}_2 = \bar{G}_R(\bar{p}_2), $$  \hspace{1cm} (41)

for the solid phase. Here

$$ \bar{F}_s(\bar{p}) = \begin{cases} \frac{\bar{A}_s}{(\bar{p} + \bar{\pi} + B_s)^{1/2}} & \text{if } \bar{p} > \bar{p}_s \text{ (shock)}, \\ \frac{2\bar{c}_s}{(\bar{\gamma} - 1)} \left[ \frac{\bar{p} + \bar{\pi}}{\bar{p}_s + \bar{\pi}} \right]^{(\bar{\gamma} - 1)/2\bar{\gamma}} - 1 & \text{if } \bar{p} < \bar{p}_s \text{ (rarefaction)}, \end{cases} $$  \hspace{1cm} (42)

and

$$ \bar{G}_s(\bar{p}) = \begin{cases} \bar{p}_s \frac{(\bar{\gamma} - 1)(\bar{p}_s + \bar{\pi}) + (\bar{\gamma} + 1)(\bar{p} + \bar{\pi})}{(\bar{\gamma} - 1)(\bar{p} + \bar{\pi}) + (\bar{\gamma} + 1)(\bar{p}_s + \bar{\pi})} & \text{if } \bar{p} > \bar{p}_s \text{ (shock)}, \\ \bar{p}_s \left( \frac{\bar{p} + \bar{\pi}}{\bar{p}_s + \bar{\pi}} \right)^{1/\bar{\gamma}} & \text{if } \bar{p} < \bar{p}_s \text{ (rarefaction)}, \end{cases} $$  \hspace{1cm} (43)

for $s = L$ and $R$, where

$$ \bar{A}_s = \frac{2}{(\bar{\gamma} + 1)\bar{p}_s}, \quad \bar{B}_s = \frac{(\bar{\gamma} - 1)}{(\bar{\gamma} + 1)}(\bar{p}_s + \bar{\pi}), \quad \bar{c}_s = \sqrt{\frac{\bar{\gamma}(\bar{p}_s + \bar{\pi})}{\bar{p}_s}}. $$  \hspace{1cm} (44)

Due to the form of the virial equation of state, it is more convenient to parameterize the velocity and pressure
of the gas in regions 1 and 2 with density. Thus, we take

$$ u_1 = u_L - F_L(p_1), \quad p_1 = H_L(p_1), \quad u_2 = u_R + F_R(p_2), \quad p_2 = H_R(p_2), $$  \hspace{1cm} (45)

where

$$ F_s(p) = \begin{cases} \left[ \frac{p_s}{p} \left( \frac{p}{p_s} - 1 \right) \left( 1 - \frac{p_s}{p} \right) \right]^{1/2} & \text{if } p > p_s \text{ (shock)}, \\ \int_{p_s}^{p} \left( c/\rho \right) d\rho & \text{if } p < p_s \text{ (rarefaction)}, \end{cases} $$  \hspace{1cm} (46)

and

$$ H_s(p) = \begin{cases} p_s \left[ 1 + \frac{b-1}{2} (1 + b p_s) \left( 1 - \frac{p_s}{p} \right) \right] & \text{if } p > p_s \text{ (shock)}, \\ p_s \left( \frac{p}{p_s} \right)^{\gamma} \left( \frac{1 + b p_s}{1 + b p_s} \right) \exp \left[ (\gamma - 1)b(\rho - p_s) \right] & \text{if } p < p_s \text{ (rarefaction)}, \end{cases} $$  \hspace{1cm} (47)
for $s = L$ and $R$. Note that the formulas for $F_s(p)$ in (46) involve the pressure $p$ which, in turn, is given by $p = H_s(p)$ in (47). Also, the evaluation of $F_s(p)$ for the rarefaction case requires a numerical quadrature. Once the states in regions 1 and 2 are found it is straightforward to determine the location of the shocks or rarefactions in the $x$-$t$ plane, see Toro [22]. The state between the solid and gas contacts with subscript 0 may be related to the state across the gas contact by the constraint that the velocity and pressure are continuous. Thus, for the configuration shown in Figure 5, we have $u_0 = u_2$ and $p_0 = p_2$. This is one of two main solution configurations. The other configuration has the solid contact to the right of the gas contact, in which case $u_0 = u_1$ and $p_0 = p_1$.

In view of the parameterizations in (41) and (45) and the constraints across the gas contact, the intermediate states in the solution of the Riemann problem depend only on the five quantities $(\rho_0, \rho_1, p_2, \bar{p}_1, \hat{p}_2)$. These quantities are determined by the jump conditions across the solid contact. For the solution configuration in Figure 5, for example, the jump conditions imply the equations

\[
\begin{align*}
\bar{u}_1 &= \hat{u}_2, \\
\alpha_L \rho_1 (u_1 - \bar{u}_1) &= \alpha_R \rho_0 (u_2 - \hat{u}_2), \\
\alpha_L \tilde{p}_1 + \alpha_L \rho_1 (u_1 - \bar{u}_1)^2 &= \alpha_R \tilde{p}_2 + \alpha_R \rho_2 (u_2 - \hat{u}_2)^2, \\
\frac{p_1}{(\gamma - 1) \rho_1 (1 + b \rho_1)} + \frac{p_1}{\rho_1} + \frac{1}{2} (u_1 - \bar{u}_1)^2 &= \frac{p_2}{(\gamma - 1) \rho_0 (1 + b \rho_0)} + \frac{p_2}{\rho_0} + \frac{1}{2} (u_2 - \hat{u}_2)^2, \\
\frac{p_2}{p_1} &= \left( \frac{\rho_0}{\rho_1} \right) \left( \frac{1 + b \rho_0}{1 + b \rho_1} \right) e^{(\gamma - 1) b (\rho_0 - \rho_1)},
\end{align*}
\]

Equation (48) is a kinematic constraint involving the velocity of the solid phase on either side of the solid contact. A balance of the mass flux of gas and the momentum on either side of the solid contact is specified by (49) and (50), respectively, while (51) and (52) state that the total enthalpy and the entropy of the gas are continuous across the solid contact. We note that the jump conditions for the opposite case when the solid contact lies to the right of the gas contact are similar to the equations above, but have the densities $(\rho_0, \rho_1)$ replaced by $(\rho_2, \rho_0)$.

The solution of the system of five equations at the solid contact may be found iteratively. The approach used here follows the one suggested in [14] which is a two-stage iterative procedure. In the first stage, it is assumed that $\alpha_L = \alpha_R$ so that the phases decouple and the intermediate states for the solid and the gas can be found separately. An iterative procedure for this follows from the discussion in [22], and results in the state $\bar{p}_1 = \hat{p}_2 = \bar{p}_s$ for which $\bar{u}_1 = \hat{u}_2 = \bar{u}_s$, and the states $\rho_1 = \rho_{1s}$ and $\rho_2 = \rho_{2s}$ for which $u_1 = u_2 = u_s$ and $p_1 = p_2 = p_s$. (The state $\rho_0$ is not needed for this first stage.) The initial choice for the second stage of the iterative procedure uses a linearization of the solid contact jump conditions about the decoupled star state computed in the first stage assuming $|\alpha_R - \alpha_L|$ is small. Let

$$\bar{p}_1 = \hat{p}_s + \delta \bar{p}_1, \quad \hat{p}_2 = \hat{p}_s + \delta \hat{p}_2, \quad \rho_1 = \rho_{1s} + \delta \rho_1, \quad \rho_2 = \rho_{2s} + \delta \rho_2,$$

and define

$$\Delta u_s = u_s - \bar{u}_s, \quad \Delta p_s = p_s - \hat{p}_s.$$

Assuming that the star states are known and that the jump in the volume fraction is small, we linearize the jump conditions to find

$$\delta \bar{p}_1 = \frac{-F'_R(\hat{p}_s) \Delta \rho_s}{F'_L(\hat{p}_s) + F_R(\hat{p}_s)} \left( \frac{\alpha_R - \alpha_L}{\alpha_m} \right), \quad \delta \hat{p}_2 = \frac{F'_L(\hat{p}_s) \Delta p_s}{F'_L(\hat{p}_s) + F_R(\hat{p}_s)} \left( \frac{\alpha_R - \alpha_L}{\alpha_m} \right),$$

and

$$\delta \rho_1 = \frac{-\rho_{ks} \Delta u_s F_R(\rho_{2s}) + H'_R(\rho_{2s}) \Delta u_s}{(1 - M_k^2) F'_L(\rho_{1s}) H'_R(\rho_{2s}) + F'_R(\rho_{2s}) H'_L(\rho_{1s})} \left( \frac{\alpha_R - \alpha_L}{\alpha_m} \right),$$

$$\delta \rho_2 = \frac{\rho_{ks} \Delta u_s F'_L(\rho_{1s}) - H'_L(\rho_{1s}) \Delta u_s}{(1 - M_k^2) F'_L(\rho_{1s}) H'_R(\rho_{2s}) + F'_R(\rho_{2s}) H'_L(\rho_{1s})} \left( \frac{\alpha_R - \alpha_L}{\alpha_m} \right),$$

where

$$M_k^2 = \left( \frac{\Delta u_s}{c_{ks}} \right)^2, \quad c_{ks}^2 = \frac{\gamma p_s}{\rho_{ks}} \left[ 1 + b \rho_{ks} - \frac{b^2 \rho_{ks}^2}{\gamma(1 + b \rho_{ks})} \right], \quad k = \begin{cases} 1 & \text{if } u_s > \bar{u}_s, \\ 2 & \text{if } u_s < \bar{u}_s, \end{cases}$$
and \(\alpha_m\) and \(\bar{\alpha}_m = 1 - \alpha_m\) are chosen intermediate volume fractions. In practice, we take \(\alpha_m\) to be the value between \(\alpha_L\) and \(\alpha_R\) closest to 0.5. The middle gas density in the linearized solution is given by

\[
\rho_0 = \rho_k + \rho_{k+} \frac{\Delta u_k \Delta u_s}{c_k^2 (1 - M_{k+}^2)} \left( \frac{\alpha_R - \alpha_L}{\alpha_m} \right).
\]

The linearized solution is well defined provided the subsonic condition is met, i.e. \(M_{k+}^2 < 1\), and neither phase vanishes. If the residual of the solid contact jump conditions for the linearized solution is sufficiently small, then this solution is accepted. If the residual is too large, then the linearized solution becomes the first guess in a full Newton iteration to obtain the solution of the jump conditions, and thus the solution of the Riemann problem.

Once the intermediates states are found, the position of shocks, rarefactions and contacts separating the various regions are computed. In particular, we are interested in the intermediate state in the region that contains the ray \(x = 0\), as well as the states on either side of the solid contact. The intermediate state along \(x = 0\) is used to compute the Godunov flux in (39), and the states on either side of the solid contact are used to compute the contributions from the nozzling terms. The full details of this numerical construction are given in [14].

### 6.2 Source step

The source step, \(\hat{U}_j = S_k(\Delta t/2)U_j\), involves a numerical integration of the system of ODEs in (38). This system of seven ODEs can be reduced to a system of four ODEs and three constraints representing conservation of mass, momentum and energy of the mixture. In fact, it is convenient to include the saturation constraint explicitly so that the set has the form

\[
\frac{d}{dt} \tilde{V} = \tilde{K}(\tilde{V}, V), \quad \tilde{V}(0) = V_0, \quad V(0) = V_0, \quad V(t) + \tilde{V}(t) = V_0 + \tilde{V}_0,
\]

where

\[
\tilde{V} = \begin{bmatrix} \tilde{\alpha} \\ \tilde{\alpha} \bar{\rho} \\ \tilde{\alpha} \bar{\rho} u \\ \tilde{\alpha} \bar{\rho} E \end{bmatrix}, \quad V = \begin{bmatrix} \alpha \\ \alpha \rho \\ \alpha \rho u \\ \alpha \rho E \end{bmatrix}, \quad \tilde{K}(\tilde{V}, V) = \begin{bmatrix} F + C/\bar{\rho} \\ C \\ M \\ E - pF \end{bmatrix}.
\]

The eight components of \([\tilde{V}_0, V_0]\) are specified by the seven components of \(U_j\) and the saturation constraint \(\alpha_j = 1 - \tilde{\alpha}_j\). The goal is to integrate the equations numerically from \(t = 0\) to \(t = \Delta t/2\). (The initial time \(t = 0\) is chosen for convenience and is taken to be the time for the input state \(U_j\).) The integration is performed using an adaptive Runge-Kutta scheme involving the following order (2,3) pair:

\[
\begin{align*}
\tilde{V}^{(2)} &= \tilde{V} + \frac{2}{9} \tilde{Z}_1 + \frac{3}{9} \tilde{Z}_2 + \frac{4}{9} \tilde{Z}_3, \\
\tilde{V}^{(3)} &= \tilde{V} + \frac{2}{9} \tilde{Z}_1 + \frac{3}{9} \tilde{Z}_2 + \frac{4}{9} \tilde{Z}_3,
\end{align*}
\]

where

\[
\begin{align*}
\tilde{Z}_1 &= \delta t \tilde{K}(\tilde{V}, V), \\
\tilde{Z}_2 &= \delta t \tilde{K} \left( \tilde{V} + \frac{1}{2} \tilde{Z}_1, V_1 \right), \\
\tilde{Z}_3 &= \delta t \tilde{K} \left( \tilde{V} + \frac{3}{4} \tilde{Z}_2, V_2 \right),
\end{align*}
\]

and \(\delta t\) is a time step on the interval \([0, \Delta t/2]\) to be chosen adaptively according to an error estimate.

The integration begins at \(t = 0\) with \([\tilde{V}, V] = [\tilde{V}_0, V_0]\) and \(\delta t = \Delta t/2\). An estimate of the truncation error is \(\| \tilde{V}^{(2)} - \tilde{V}^{(3)} \|/\delta t\), and if this estimate is below a tolerance, then the step is accepted and the components of \(\hat{U}_j = S_k(\Delta t/2)U_j\) are taken from the components of \([\tilde{V}^{(3)}, V^{(3)}]\). If, on the other hand, the estimate is greater than the tolerance, then \(\delta t\) is reduced and a new Runge-Kutta integration step is
performed. Again, an estimate of the error is made and checked against the tolerance in order to determine whether this step is accepted. Ultimately, it is possible for several integration steps to be taken to reach $t = \Delta t/2$ with the constraint that the error estimate is less than the tolerance at each step. This approach leads to an accurate numerical integration of the system of ODEs, but in practice the number of steps is never more than 2 or 3, since we use the estimate of the error to guide the refinement of the grid in both space and time according to a scheme of adaptive mesh refinement as we discuss below.

6.3 Adaptive mesh refinement and grid convergence

Solutions of the two-phase equations possess shocks and contacts, as noted previously, in addition to thin layers in which reaction and the relaxation processes of compaction, drag and heat transfer are important. In order to resolve these layers and to handle shocks and contacts with numerical efficiency, we use a scheme of adaptive mesh refinement (AMR) similar to that discussed in [15]. For each calculation a base grid is selected for an interval $x \in [0, L]$, say, with $\Delta x_1 = L/N$, where $N$ is the number of grid cells. The time step, $\Delta t_1$, for the base grid is selected according to the CFL stability constraint

$$\Delta t_1 = \frac{\kappa \Delta x_1}{\lambda_{\text{max}}}, \quad \lambda_{\text{max}} = \max_{1 \leq i \leq 7, 1 \leq j \leq N} |\lambda_{i,j}|,$$

where $\lambda_{i,j}$, $i = 1, \ldots, 7$, are the eigenvalues of the system given by (40) evaluated at $U^n_j$, and $\kappa$ is the CFL number taken to be 0.8 for all calculations. As the solution evolves, refinement may be required to resolve small scales in space or time. Thin layers in space are detected by flagging cells where the magnitude of the second undivided difference of the components of $U^n_j$ is larger than a tolerance. Rapid temporal variations are flagged by monitoring the number of sub-CFL time steps needed for the integration of the source term. If more than 2 or 3 integration steps are taken for a cell, then that cell is flagged for refinement. Once all cells have been checked, then refinement grid patches are constructed containing the flagged cells. A conservative interpolation scheme is used to transfer the grid data from the base grid to the refined grid patches which have spacing $\Delta x_2 = \Delta x_1/n_r$, where the refinement factor $n_r$ is taken to be 4. The time step for the refined grid patches is decreased accordingly, i.e. $\Delta t_2 = \Delta t_1/n_r$, so that the CFL stability constraint is satisfied for the refined grid patches. The process of refinement is recursive so that the refined grids at level $l < l_{\text{max}}$ may themselves be refined by a factor $n_r$ in both space and time according to the refinement criteria.

Figure 6: Grid convergence for $l_{\text{max}} = 2, 3, 4$ and 5. Behavior of (a) reaction rate (solid curves) and drag (dashed curves), and (b) compaction rate (solid curves) and heat transfer (dashed curves) for $\sigma = 10$, $p_{\text{ign}} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $H = 0.2$. The reaction rate is scaled by a factor of 5 for illustration purposes.

The convergence of numerical solutions on the AMR-grid system may be judged by comparing solutions
on a fixed based grid using increasing values for \( l_{\text{max}} \). Of particular interest for the work here are steady detonation waves and the well-resolved behavior of reaction and relaxation of the two-phase model within the structure of the detonations. Figure 6 shows profiles of reaction, drag, compaction and heat transfer for a steady detonation with upstream conditions given in Table 2 and with source parameters discussed in Section 7.1.4 for the case \( \sigma = 10 \) (see also Figure 16). The rates of reaction and compaction are given by (12) and (13), respectively, while the drag is computed using \( \delta (w - \bar{w}) \) and the heat transfer is computed using \( \mathcal{H}(T - \bar{T}) \). The calculations in the figure are performed on a base grid with \( \Delta x_1 = 0.04 \) and with up to \( l_{\text{max}} \) levels of refinement. Here we note the reaction zone and the layers of relaxation are well resolved when \( l_{\text{max}} \) equals 4 or 5. For the case \( l_{\text{max}} = 4 \) the grid spacing is \( \Delta x_4 = 0.000625 \) (corresponding to \( \Delta x_4 = 0.00469 \text{ mm} \) ) on the finest level and 440 grid cells cover the full width of the detonation structure \( \xi \in [-0.275, 0] \) shown in the figure. The convergence behavior shown in Figure 6 is for a steady reaction-led detonation. A similar behavior is obtained for compaction-led detonations, and unless noted otherwise the subsequent calculations for all cases employ this level of grid refinement. It is worth noting that the level of refinement employed here is much finer than that used in previous numerical studies. For example, the calculations in [1] used uniform grids with grid spacings similar to that of the base grid (i.e. \( l_{\text{max}} = 1 \) ) for the example shown in Figure 6. Coarser grids are also used for the calculations in [6], but these were shown to give reasonable convergence for the governing equations and parameter set considered in that paper.

7 Numerical Results

Our primary interest is in the structures of the steady detonations admitted by the model, in the dependence of these structures on the model parameters, and in the evolutionary processes leading to these structures. In order to arrive at the steady waves numerically, we consider the long-time behavior of a time-dependent piston problem. It is assumed that the explosive occupies the interval \( x \in [0, L] \), where \( L \) is large enough so that a steady wave develops on the interval. It is convenient to compute the solution of the problem in the frame of the piston. Thus, we take the initial velocity to be \( u(x, 0) = \bar{u}(x, 0) = -u_p \), where \( u_p > 0 \) is the piston velocity, and consider the impact of the explosive against a solid wall (the piston face) at \( x = 0 \). The boundary conditions at \( x = 0 \) consist of an even reflection for all of the components of \( \mathbf{u} \) in the governing equations except the momentum which is taken to be an odd reflection. (The boundary conditions at \( x = L \) are \( \partial \mathbf{u} / \partial x = 0 \) which is an outflow condition.) For all calculations, we report results for \( u_p = 0.013318 \) which corresponds to the dimensional piston velocity

\[
 u_p' = 100 \text{ m/s}.
\]

This choice provides a low-speed impact sufficient to generate an unsupported detonation for the range of parameters considered.

We remark that the long-time structure of the detonation was found to be independent of the piston velocity over a broad range appropriate for unsupported detonations. The implication is that these steady solutions are stable. It is possible that unstable steady solutions exist, but the computational approach is not capable of finding such solutions. Unsteady, long-time solutions may also exist, but none were found in the parameter domain examined.

We study the long-time steady solution, and the approach to it, for a range of parameters of the model including the reaction rate prefactor \( \sigma \), the ignition pressure \( p_{\text{ign}} \), the drag coefficient \( \delta \), the compaction viscosity \( \mu_c \), and the heat transfer coefficient \( \mathcal{H} \). The general course of this study begins by selecting nominal values for \( \delta \), \( \mu_c \) and \( \mathcal{H} \), and considering the behavior of solutions as \( \sigma \) is increased from zero with \( p_{\text{ign}} \) held fixed. This leads to a description of a family of steady near-CJ detonations, and the identification of two basic detonation structures, compaction-led and reaction-led, as mentioned in Section 1. Next, we examine the consequence of changing \( p_{\text{ign}} \), and then proceed to vary the three relaxation parameters \( \delta \), \( \mu_c \) and \( \mathcal{H} \), in turn, to study their effect while holding the reaction-rate parameters fixed. For each case with \( \sigma > 0 \), and with the upstream state and equation-of-state parameters listed in Tables 2 and 3, respectively, we find that the end state of the detonation lies on the weak branch of the fully-reacted Hugoniot very close to the CJ state. We also consider numerically the approach to the asymptotic limits of large drag and rapid compaction.
Figure 7: Evolution to a steady reactionless compaction wave for $\sigma = 0$, $\mu_c = 0.05$, $\delta = 20$ and $\mathcal{H} = 0.2$. Behavior of (a) solid volume fraction, (b) pressures $\bar{p} - \beta$ (solid curves) and $p$ (dashed curves), (c) solid and gas velocities, (d) solid and gas temperatures, (e) solid density, and (f) gas density for $t = 40, 80, \ldots, 360$.

7.1 Effect of variation of the reaction rate

The reaction rate, defined in (12), is parameterized by the prefactor $\sigma$ and the ignition pressure $p_{\text{ign}}$, and we consider each in turn. In order to study the effect of varying these parameters, we require a choice for the relaxation parameters. We take, as a base case,

$$\delta = 20, \quad \mu_c = 0.05, \quad \mathcal{H} = 0.2.$$
Using the reference scales in Table 1, the corresponding dimensional quantities are
\[
\delta' = 7.55 \times 10^9 \text{ kg/ (m}^3 \text{s)} , \quad \mu'_c = 1.07 \times 10^3 \text{ Pa s}, \quad \mathcal{H}' = 1.81 \times 10^{11} \text{ J/ (Km}^3 \text{s)}.
\]

The values for \(\delta'\), \(\mu'_c\) and \(\mathcal{H}'\) used here are similar to those discussed elsewhere, see Table 4, except for \(\mathcal{H}'\) which is larger. We choose a larger value for \(\mathcal{H}'\) so that the phase temperatures equilibrate at a reasonable distance in the tail of the steady detonation structure. We consider a range of values of \(\sigma\) and two values for \(p_{\text{ign}}\). For most of the calculations, we set \(p_{\text{ign}} = 1.4 \times 10^{-5}\), which is a value slightly greater than the dimensionless upstream gas pressure \(p_0 = 1.1843 \times 10^{-5}\) listed in Table 2. This choice switches the reaction on even when compaction is quite weak. Later, in Section 7.1.6, we consider the behavior for a value of \(p_{\text{ign}}\) which is 10 times greater.

Figure 8: Wavefront behavior for \(\sigma = 0, 1, 2, 4\) and 10 with \(p_{\text{ign}} = 1.4 \times 10^{-5}\), \(\mu_c = 0.05\), \(\delta = 20\) and \(\mathcal{H} = 0.2\): (a) wave paths in the \(x-t\) plane and (b) wave velocity versus time. (Positions and velocities are given in the piston frame of reference.)

### 7.1.1 Inert compaction for \(\sigma = 0\)

Figure 7 shows the time-dependent behavior of the solution for \(\sigma = 0\) when the reaction is off completely. The piston generates a compaction wave, and this wave propagates away from the piston face at a velocity which approaches a steady value of 0.0377 in the frame of the piston. This velocity corresponds to a dimensional value of 383.4 m/s in the laboratory frame of reference, a value significantly smaller than \(D'_{\text{CJ}} = 7508.8\) m/s.

The value of \(\bar{\alpha}\) rises from its upstream value \(\bar{\alpha}_0 = 0.73\) through the wave to an asymptotic value equal to 0.987 far downstream (see Figure 7(a)). The behavior of the solid pressure offset by the configuration pressure \(\bar{p} - \beta\) (solid curves) and the gas pressure \(p\) (dashed curves) are shown in Figure 7(b). Here we see a rise in both pressures, to a greater extent in \(\bar{p} - \beta\), at the front of the compaction wave, followed by a decrease in \(\bar{p} - \beta\) towards an equilibrium value of \(\bar{p} - \beta = \bar{p} = 3.4 \times 10^{-4}\), approximately. While the profiles of \(\bar{p} - \beta\) each have a local maximum, the corresponding profiles of the solid pressure alone (not shown) increase monotonically to a maximum value at the piston face. There, the dimensional values for the gas and solid pressures approach the equilibrium values of \(p' = 7.24\) MPa and \(\bar{p}' = 59.1\) MPa, respectively. For the value of \(\mu_c\) chosen the width of the steady compaction zone is approximately 15 dimensionless units of length, corresponding to 113 mm. The phase velocities and temperatures, shown in Figures 7(c) and 7(d), respectively, are in equilibrium throughout the compaction wave. (The velocity and temperature for both phases are plotted but only one family of curves is visible in each figure.) Finally, the compaction creates an increase in density of both phases, as expected, with only a small increase in the solid density as compared to the gas density (see Figures 7(e) and 7(f)). (There is a drop in density and an increase in temperature...
near the piston face which is due to a start up error created by the discontinuity in the initial conditions at $x = 0$.) We note that the structure of the steady compaction wave found here is qualitatively similar to that computed by Gonthier and Powers [6], and the viscous structure computed by Powers (c.f. case E in [16]). Also, the dimensional values of the wave velocity and equilibrium pressure of the solid at the piston face are close to those observed experimentally by Sandusky and Liddiard [23].

Figure 9: Evolution to a steady detonation wave for $p_{\text{ign}} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $\mathcal{H} = 0.2$. Behavior of the solid volume fraction for (a) $\sigma = 1$, (b) $\sigma = 2$, (c) $\sigma = 4$, and (d) $\sigma = 10$.

7.1.2 Transition to detonation for $\sigma > 0$

When $\sigma > 0$, the reaction switches on and a transition from the slow compaction wave into a fast detonation occurs in due course. Figure 8 illustrates the general trend of this transition for the cases $\sigma = 1, 2, 4$ and 10. For each case the wave in the $x$-$t$ plane begins as a slow compaction wave which follows the path of the nonreactive case $\sigma = 0$. At later times, transitions to fast waves of reaction occur, and the times of the transitions decrease with increasing $\sigma$. Once a transition occurs, the speed of the detonation (in the laboratory frame of reference) ultimately approaches a value approximately equal to 1 which is the dimensionless CJ detonation velocity. (The value approached in the graph is $1 - u_p = 0.9867$ for the piston frame.) The corresponding behavior of the volume fraction of the solid, displayed in Figure 9 for each value of $\sigma$, shows an early rise in $\bar{\alpha}$ due to compaction but then a transition to detonation with an ultimate decrease in $\bar{\alpha}$ to zero as the solid phase is consumed by the reaction. For $\sigma = 1, 2$ and 4, the profiles of the steady detonation waves include a thin compaction layer at the front. For $\sigma = 10$ there is no apparent compaction layer; it has been eroded by the strong reaction. The width of the steady detonation profiles decrease with increasing $\sigma$.

The presence or absence of a thin compaction layer in the front of the detonation profile is one dis-
tistinguishing feature of the two basic steady detonation structures found in our numerical study. The cases \( \sigma = 4 \) and \( \sigma = 10 \) are representative of these two structures, compaction-led and reaction-led detonations, respectively, and we now consider these two cases in detail. In particular, we focus on the time-dependent behavior during the transition to detonation for each case, and also on the structure of the long-time steady detonations.

Figure 10: Reaction-induced modification of inert compaction (\( \sigma = 0 \)) for \( \sigma = 4 \). Other parameters are \( p_{\text{ign}} = 1.4 \times 10^{-5}, \ \mu_c = 0.05, \ \delta = 20 \) and \( \mathcal{H} = 0.2 \). Profiles of (a) solid (solid curves) and gas (dashed curves) velocities, (b) solid (solid curves) and gas (dashed curves) pressures, (c) solid volume fraction and (d) drag (solid curve) and nozzling (dashed curve) contributions to momentum exchange, at a very early time, \( t = 9 \).

7.1.3 Compaction-led detonation for \( \sigma = 4 \)

Figures 10–12 display the details of the process of compaction-to-detonation transition for the case \( \sigma = 4 \). Figure 10 shows the ways in which the inclusion of reaction disturbs the inert compaction profiles at an early time, \( t = 9 \). In the absence of reaction the inert solution displays drag-induced velocity equilibrium over the entire profile (see Figure 10(a)), a reduced solid pressure \( \bar{p} - \beta \) that is in excess of the gas pressure \( p \) (see Figure 10(b)), and the resulting monotonic compaction profile (see Figure 10(c)). With reaction included, a dip in the solid volume fraction near the piston face signals conversion of solid into gas (see Figure 10(c)). The gas so generated disturbs the state of velocity equilibrium (see Figure 10(a)); it moves faster than, and attempts to permeate into, the solid. However, the depth of permeation permitted by the solid is narrow, and the resulting confinement serves to raise the pressure of the gas (see Figure 10(b)). Figure 10(d) shows that by far, the principal contributor to the transfer of momentum from the gas to the solid is drag; nozzling plays a minor role at this time, while the reaction-rate contribution (not shown) is negligible on the scale.
of these plots. Within the reaction zone this momentum exchange accelerates the solid to velocities above those present in inert compaction (see Figure 10(a)) and also raises its pressure (see Figure 10(b)). This disturbance in the state of the solid is conveyed acoustically into the region upstream of the reaction zone, elevating the pressure of the solid there to levels above those existing in the inert case. The elevated pressure, in turn, induces a larger compaction (see Figure 10(c)), which accelerates the gas by squeezing it out of the pores of the solid, and thus dragging the solid with it.

Figure 11: Evolution of reactive wave for $\sigma = 4$, $p_{\text{ign}} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $H = 0.2$. Profiles of (a) solid (solid curves) and gas (dashed curves) velocities, (b) reduced solid (solid curves) and gas (dashed curves) pressures, (c) solid volume fraction, and (d) contributions of drag (solid curve), reaction (dashed curves) and nozzling (chain-dashed curves) to momentum exchange, at $t = 9.4$, $9.8$ and $10.2$.

Figure 11 displays early evolution of reactive solution profiles close to the piston face, at $t = 9.4$, $9.8$ and $10.2$. The increased gas pressure, already seen at $t = 9$, accelerates the reaction rate, which in turn increases the rate of gas production and hence a further elevation in gas pressure. Thus these later-time profiles are essentially amplified versions of those at $t = 9$, but with three additional features. First, the rapid increase in gas pressure leads to the development of a gas shock, clearly incipient at $t = 10.2$ in Figure 11(a). In fact, the gas shock plays the role of the leading edge of the reaction zone. Second, beginning at $t = 9.8$, the solid velocity near the piston face is seen to overtake the gas velocity, thus reversing the sign of the drag term (see Figure 11(a) and 11(d)). This reduction in gas velocity is the result of the high-pressure gas pushing backwards towards the piston face. Third, Figure 11(d) shows that while drag still provides the largest contribution in magnitude to the momentum exchange from gas to solid, it does so in an increasingly narrow domain behind the gas shock. The nozzling contribution, active throughout the reaction zone, has now grown to substantial levels comparable to drag, while the contribution due to reaction, though discernible and growing, remains small and negative. We also note, from Figure 11(c), that the increased solid pressure upstream of the reaction zone continues to generate higher levels of compaction there.
Figure 12: Transition from compaction wave to compaction-led detonation for $\sigma = 4$, $p_{\text{ign}} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $H = 0.2$. Profiles of (a) solid volume fraction, (b) rates of compaction (solid curves) and reaction (dashed curves), (c) velocity of solid (solid curves) and gas (dashed curve), (d) pressures $\bar{p} - \beta$ (solid curves) and $p$ (dashed curves), and (e) temperatures of solid (solid curves) and gas (dashed curves) for $t = 9.0, 9.4, \ldots, 13.0$. (The reaction rate is scaled by a factor of 5 for illustration purposes.)

Figure 12 shows the final evolution of the solution during the transition to a compaction-led detonation. As the solution advances and the reaction builds in strength, Figures 12(c) and 12(d) show a rapid growth in the strengths of both the shock in the gas and the pressure pulse in the solid. Concurrently, there is an increase in the rate of compaction and a resulting sharp increase in the solid volume fraction; see Figure 12(a). Figures 12(a), 12(c) and 12(d) also show the formation of a solid shock, at $t = 10.6$ approxi-
mately, at the head of the growing compaction layer. Velocity equilibrium is approached nearly everywhere (see Figure 12(d)), except in a narrow region behind the gas shock. Pressure equilibrium is approached nearly everywhere as well, except in the region between the two shocks. Figure 12(b) shows growth in both the reaction rate and the rate of compaction, the former with the gas shock as the leading edge and the latter confined to the region between the two shocks at later times. A sharp peak in the gas temperature can be seen behind the gas shock (see Figure 12(e)). Later, a rapid rise in the gas and solid temperatures ahead of the sharp peak occurs as a result of the formation of the shock in the solid phase. For the case with \( \sigma = 4 \), the compaction layer leading the detonation, which forms during transition, persists in the long-time steady solution as seen earlier in Figure 9(c).

![Figure 13](image-url) Figure 13: Profiles of the momentum exchange terms for \( \sigma = 4, \ p_{\text{ign}} = 1.4 \times 10^{-5}, \ \mu_c = 0.05, \ \delta = 20 \) and \( H = 0.2 \): force (per unit volume) due to drag (solid curves), reaction (dashed curves) and nozzling (chain-dashed curves) at \( t = 10.6, 11.0, \ldots, 13.0 \).

Figure 13 shows profiles of the momentum exchange terms due to drag, compaction and reaction. The salient feature of these profiles is the growth in the contribution of momentum exchange due to reaction, which nearly fully cancels the nozzling contribution, leaving the thin spike in drag as the sole momentum exchange mechanism in the fully-established wave.

The structure of the long-time steady detonation for the case \( \sigma = 4 \) is shown in Figure 14. The plots in the figure are made in the frame of the steady wave, and are given in terms of the independent variable \( \xi = x - D t \), where \( \xi = 0 \) is taken as the leading edge of the detonation. The end of the detonation structure, plotted at the left boundary in each profile, is taken to be the point corresponding to \( \bar{\alpha} = .001 \). For \( \sigma = 4 \), we see a thin compaction layer leading the steady wave as noted previously and as shown in Figure 14(a). The rates of reaction, compaction and drag for this profile, given by (12), (13) and \( \delta (u - \bar{u}) \), respectively, are shown in Figure 14(b). In this plot, we note a spike in the rate of compaction ahead of the main reaction zone. There is also a very thin layer in which drag is significant at the beginning of the reaction zone. This is caused by the rapid production of gas in the early portion of the reaction zone, which, in turn, triggers a disequilibrium in the relative phase velocities (see Figure 14(c)) as mentioned earlier. This difference is short lived, however, and the phase velocities soon return to equilibrium. The magnitude of the rate of heat transfer is very small relative to the rates shown and is not plotted. In Figure 14(d), we plot the (base 10) logarithm of the Mach numbers \( |M| = |\bar{w}/\bar{c}| \) and \( |M| = |w/c| \), where we recall that \( \bar{w} = \bar{u} - D, \ w = u - D \), and the sound speeds \( \bar{c} \) and \( c \) are defined in (11). This plot shows that the detonation profile indicative of this basic structure begins with a shock in the solid phase at \( \xi = 0 \), where the \( |M| \) crosses 1, followed by a layer of compaction. (The Mach numbers ahead of the leading shocks are much greater than 1.) The compaction layer ends at a gas shock located at \( \xi = -0.090 \) where \( |M| \) crosses 1, and this event signals the start of significant reaction and the brief layer of velocity disequilibrium. As the reaction proceeds, the flow accelerates smoothly, passing through \( |M| = 1 \) at \( \xi = -0.827 \) which corresponds to a removable singularity of the system of ODEs for the steady equations, and proceeding to an end state which is slightly supersonic. This suggests that the end state lies on the weak branch of the fully-reacted Hugoniot, which is confirmed.
Figure 14: Steady compaction-led detonation structure for $\sigma = 4$, $p_{\text{ign}} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $H = 0.2$. Profiles of (a) volume fractions, (b) rates of reaction, compaction and drag, (c) phase velocities relative to the steady wave, (d) phase Mach numbers, (e) phase pressures, and (f) phase temperatures. (The reaction rate is scaled by a factor of 5 for illustration purposes.)

by the plot in Figure 17 as discussed below. Profiles of pressure and temperature are shown in Figures 14(e) and 14(f), respectively, and these illustrate the mechanical and thermal disequilibrium between the phases in this compaction-led structure. The largest difference in pressure occurs in the compaction layer near the front of the detonation, while a large difference in temperature occurs throughout most of the structure, and in particular behind the gas shock where there is a spike in the gas temperature, equal to 0.29 which corresponds to 6800 K approximately. We note that while $\bar{\rho} - \beta$ is plotted together with $p$ to illustrate
mechanical equilibrium or disequilibrium, the configuration pressure $\beta$ is much smaller than $\bar{p}$ behind the leading shock in the detonation so that $\bar{p} - \beta \approx \bar{p}$ in Figure 14(e) and the subsequent plots of pressure.

Figure 15: Transition from compaction wave to reaction-led detonation for $\sigma = 10$, $p_{\text{ign}} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $H = 0.2$. Profiles of (a) solid volume fraction, (b) rates of compaction (solid curves) and reaction (dashed curves), (c) velocity of solid (solid curves) and gas (dashed curve), (d) pressures $\bar{p} - \beta$ (solid curves) and $p$ (dashed curves), and (e) temperatures of solid (solid curves) and gas (dashed curves) for $t = 4.4, 4.6 \ldots, 6.0$. (The reaction rate is scaled by a factor of 5 for illustration purposes.)
7.1.4 Reaction-led detonation for $\sigma = 10$

We now turn our attention to the behavior of the solution during transition from compaction wave to reaction-led detonation for the case $\sigma = 10$. The solution is shown in Figure 15, and these plots may be compared to the ones shown previously for the compaction-led case in Figure 12 for $\sigma = 4$. The early behavior for the present case, characterized by the formation of a gas shock and a compaction layer ahead of it, is similar to the previous case. As before, a shock in the solid phase forms in the front of the compaction layer, but now the relative velocity of the gas shock behind it is larger due to the stronger reaction rate for the present case with $\sigma = 10$. As a result, the gas shock overtakes the solid shock leading to a collapse of the compaction layer (see Figures 15(a) and (b)). By the end of the transition, the gas shock is seen at the front of the detonation with the main reaction zone following immediately behind it. By this time, the shock in the solid phase has taken a position just behind the shock in the gas phase as may be seen by the jumps in the phase velocities shown in Figure 15(c) at $t = 6.0$. At the front of the wave, there is a wide layer of velocity disequilibrium while the pressures are nearly equilibrated. A large spike in the gas temperature is seen behind the leading gas shock.

The corresponding long-time steady profiles for this reaction-led detonation structure are shown in Figure 16. Here, as noted previously, there is no compaction layer at the leading edge of the detonation. Instead, a gas shock appears at the start of the detonation at $\xi = 0$, which is followed by a shock in the solid phase at $\xi = -0.016$. Significant reaction occurs immediately following the leading gas shock and the rate of compaction is negative due to the high gas pressure in this region. After the shock in the solid phase, the compaction rate flips sign but its magnitude remains small relative to the magnitude of the reaction rate. The region of velocity disequilibrium is significantly larger than that observed in the previous compaction-led detonation structure due to the stronger production of gas in the reaction zone for this case. As in the previous steady structure, there is a smooth passage through $|M| = 1$ to a slightly supersonic end state on the weak branch of the fully-reacted Hugoniot (see Figure 17). The plots of velocity, pressure and temperature for this case show large regions of kinematic, mechanical and thermal disequilibrium in the detonation structure. This suggests that reduced two-phase models which assume some form of equilibrium between phases, such as the velocity and pressure equilibrium models discussed in [10, 11], may produce results with significant error for this case. Even for smaller values of the reaction rate, such as the $\sigma = 4$ case discussed previously, the regions of disequilibrium are not negligible and play a role in the structure of the detonation profiles.

7.1.5 End-state behavior for $\sigma = 4$ and 10

Figure 17(a) shows the fully-reacted Hugoniot for the upstream state and the equation-of-state parameters given in Tables 2 and 3, respectively. The mixture Rayleigh line, given by (26), is shown for the case $D = D_{CJ} = 1$. The CJ speed is a close approximation to the detonation velocities found for the positive values of $\sigma$ computed. The exact CJ state is marked on the graph for reference, and this may be compared with the marks corresponding to the end states obtained from the numerical detonation structures for $\sigma = 4$ and 10. Here, as noted previously, we see that the computed end states lie on the weak branch of the exact fully-reacted Hugoniot very close to the CJ state. The detonation velocities in the laboratory frame for the cases with $\sigma = 4$ and $\sigma = 10$ are $D = 1.0040$ and 1.0013, respectively. Figure 17(b) shows the profiles of the mixture pressure in the corresponding steady waves, with the end states identified in each case. These profiles simply show that even though the end state lies on the weak branch of the fully-reacted Hugoniot, the wave is not 'weak' in the classical, one-phase sense. Rather, these are analogous to the eigenvalue detonations that correspond to an endothermic/exothermic reaction pair or weak curvature [19].

It is instructive to compare these results to those of Gonthier and Powers [6], who also construct steady solution as the limit of a piston-impact problem, for a model that has a different reaction scheme and does not contain the nozzling terms. Their velocity profiles are similar to our reaction-led case but the pressure profiles are not in that we show a broad region of pressure disequilibrium while they do not. We find that the solid temperature rises monotonically in the wave, while their temperature profile has a hump and the reaction zone terminates with a nonzero slope. Their solid velocity is supersonic throughout while we have a solid shock. However, they also have a slightly supersonic gas velocity at the end state.
Figure 16: Steady reaction-led detonation structure for $\sigma = 10$, $p_{\text{ign}} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $H = 0.2$. Profiles of (a) volume fractions, (b) rates of reaction, compaction and drag, (c) phase velocities relative to the steady wave, (d) phase Mach numbers, (e) phase pressures, and (f) phase temperatures. (The reaction rate is scaled by a factor of 5 for illustration purposes.)

7.1.6 Effect of varying $p_{\text{ign}}$

As already remarked, the low value of $p_{\text{ign}}$ employed so far causes the reaction to be switched on even for weak compaction. We now consider $p_{\text{ign}} = 14 \times 10^{-5}$, which is 10 times greater than the value used in the previous calculations, and set $\sigma = 4$. Figure 18 shows the resulting evolutionary process, and it is instructive to compare these results with those of Figure 12 corresponding to the smaller $p_{\text{ign}}$. As expected, the larger ignition pressure results in a longer ignition delay, so that reaction is now triggered at a more highly
Figure 17: (a) The fully-reacted Hugoniot, mixture Rayleigh line for $D = D_{CJ} = 1$, theoretical CJ state (circle), and the computed end states for $\sigma = 4$ and 10; and (b) profiles of the mixture pressure and end states for $\sigma = 4$ (diamond) and $\sigma = 10$ (square) using $p_{ign} = 1.4 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $\mathcal{H} = 0.2$.

compacted state relative to that for the smaller value of $p_{ign}$. The higher level of compaction generates a more vigorous reaction, and hence a more rapid transition to detonation, subsequent to the delayed ignition. Once significant reaction begins the compaction wave simply provides a 'quasi-steady' initial state on which the detonation develops, and the long-time steady behavior is not significantly affected by the induction delay.

### 7.2 Solution behavior for varying relaxation parameters

We now consider the behavior of the solutions as the relaxation parameters are varied. For this study, we hold the reaction-rate parameters fixed at $\sigma = 4$ and $p_{ign} = 1.4 \times 10^{-5}$. A majority of the discussion concerns variations in the drag parameter $\delta$ and the compaction viscosity $\mu_c$ followed by a brief comment on variation in the heat transfer coefficient $\mathcal{H}$. The effect on the steady structure, as well as that on the evolution, is addressed. Values for these parameters are difficult to measure experimentally, and while general parameters ranges have been suggested in the literature (see Table 4), well-resolved solutions of the model have not yet been reported for a broad range of parameter values. It is hoped that the trends that are revealed here will provide a guide to choosing the relaxation parameters.

We begin by setting $\mathcal{H} = 0.2$, and varying either $\delta$ or $\mu_c$, while holding the other one fixed. It is found that in general, smaller values of $\delta$ and $\mu_c$ favor steady reaction-led detonation structures, while larger values lead to steady compaction-led structures. The detonation velocity $D$ is close to $D_{CJ}$ for all values of the relaxation parameters considered. Figure 19, the result of extensive numerical exploration, shows the boundary $\delta = \delta^*(\mu_c)$, or $\mu_c = \mu_c^*(\delta)$ in the $\delta$ - $\mu_c$ plane separating the two regions. It is found that the change from one steady structure to the other occurs abruptly across the boundary. Consider, for example, $\mu_c = 0.05$, for which $\delta^*$ is approximately 13.2. Figure 20 shows steady profiles for two nearby values of $\delta$, $\delta = 13.0$ and $\delta = 13.5$, that straddle the boundary. We see immediately from the compaction profiles in Figure 20(a) that $\delta = 13.0$ results in a reaction-dominated wave and $\delta = 13.5$ in a compaction-dominated wave. Predictably, the larger $\delta$ has a narrower zone of velocity disequilibrium (see Figure 20(c)), but the extent of narrowing associated with the small change in $\delta$ is striking. Correspondingly large changes also appear in the pressure profiles in Figure 20(d) and in the compaction, drag and reaction-rate profiles in Figure 20(b).

#### 7.2.1 Effect of varying $\delta$

Figure 21 illustrates the behavior for values of $\delta$ less than $\delta^*$ for $\mu_c = 0.05$. The overall behavior for these values is similar to that of the reaction-led structure shown previously in Figure 16, and changes with $\delta$
Figure 18: Transition from compaction wave to compaction-led detonation for $\sigma = 4$, $p_{\text{ign}} = 14 \times 10^{-5}$, $\mu_c = 0.05$, $\delta = 20$ and $H = 0.2$. Profiles of (a) solid volume fraction, (b) rates of compaction (solid curves) and reaction (dashed curves), (c) velocity of solid (solid curves) and gas (dashed curve), (d) pressures $\bar{p} - \beta$ (solid curves) and $p$ (dashed curves), and (e) temperatures of solid (solid curves) and gas (dashed curves) for $t = 66.4, 66.8, \ldots, 70.4$. (The reaction rate is scaled by a factor of 5 for illustration purposes.)

more gradual, as indicated by the compaction profiles of Figure 21(a). As $\delta$ increases the layer of velocity disequilibrium narrows (see Figure 21(c)). There is an associated decrease in the width and an increase in the vigor of the reaction zone (see Figures 21(a) and 21(b)), which in turn, results in higher gas pressures (see Figure 21(d)). Also, we note that for small values of $\delta$, such as for $\delta = 2$, there is no shock in the solid behind the leading gas shock, but rather a smooth compression as seen, for example, in the plot of the
solid velocity (see Figure 21(c)). As \( \delta \) increases the smooth compression becomes a shock in the solid phase characteristic of the strong reaction-led detonation structure described in the previous section.

The behavior of the steady compaction-led detonations for values of \( \delta \) greater than \( \delta^* \) is shown in Figure 22. Here we shall also track the asymptotic approach to any limiting behavior as \( \delta \) becomes large while the other parameters are held fixed. In Figure 22(a) we see very little change in the behavior of the volume fractions, indicating that the rather large variation in \( \delta \) has a weak effect on the width of the compaction layer, see also Figure 22(b). For this range of \( \delta \), the changes in the steady behavior occur near the end of, and behind, the compaction layer. In Figure 22(b) we note that for \( \delta = 13.5 \) and 20 there is a gas shock leading the main reaction zone, but for larger values of \( \delta \) this shock weakens and disappears as the layer of velocity disequilibrium shrinks. The rate of drag given by \( \delta(w - \bar{w}) \) approaches an \( O(1) \) asymptotic behavior in agreement with the analysis described by Kapila et. al in [10]. The behavior of the solid pressure, \( \bar{p} - \beta \), shown in Figure 22(d), shows little change in accordance with the behavior of the compaction layer, and the gas pressure changes only near the end of the layer and appears to approach a smooth asymptotic behavior.

It is worth noting that while the layer of velocity disequilibrium shrinks as \( \delta \) increases, the larger values of \( \delta \) (holding the other parameters fixed) favor the compaction-led detonation structure which has a relatively broad layer of pressure disequilibrium.

It is instructive to examine the effect of changing \( \delta \) on the transition time, i.e., the time at which the reactive wave peels away from the compaction wave; see Figure 8(a) for the analogous situation for varying \( \sigma \). One finds that variation of \( \delta \) provokes little change, and that in the \( x-t \) plane, trajectories of the reactive wave (not displayed) for various \( \delta \) are essentially coincident.

### 7.2.2 Effect of varying \( \mu_c \)

We now consider the effects of varying the compaction viscosity \( \mu_c \). For this study we set \( \mathcal{H} = 0.2 \) as before, and take \( \delta = 15 \). We begin with a relatively large value for \( \mu_c \) for which the compaction rate \( F \) given by (2) is relatively weak, and consider the behavior as \( \mu_c \) decreases so that the compaction rate strengthens. As already stated, larger values of \( \mu_c \) favor compaction-led detonation structures with relatively wide layers of compaction, while reaction-led structures are obtained for smaller values of \( \mu_c \). Again there is an abrupt change between the two basic steady structures across the boundary \( \mu_c^*(\delta) \). For values of \( \mu_c \) just below \( \mu_c^* \) we find that the time evolution begins with a transition from compaction wave to compaction-led detonation similar to that shown in Figure 12, and while the compaction-led detonation appears to be steady, a second transition occurs to a fully-steady reaction-led detonation at later times. The second transition, as we
Figure 20: Steady reaction-led detonation structures for $\sigma = 4$, $\mu_c = 0.05$, $H = 0.2$ and $\delta = 13$ and $13.5$. Profiles of (a) volume fractions, (b) rates of reaction, compaction and drag, (c) phase velocities relative to the steady wave, and (d) phase pressures $\bar{p} - \beta$ (solid curves) and $p$ (dashed curves). (The reaction rate is scaled by a factor of 5 for illustration purposes.)

illustrate below, is delicate and requires a very fine grid to capture it accurately. For smaller values of $\mu_c$, the second transition occurs sooner (similar to that seen in Figure 15), and we note the asymptotic approach to pressure equilibration resulting from a very rapid compaction rate. As before, we focus our attention near the front of the steady detonation structures where the solution of the two-phase model shows the greatest change.

The compaction-led detonation structures for $\mu_c = 0.025$, 0.02 and 0.015, all greater than $\mu_c^*$, are shown in the set of plots in Figure 23. As $\mu_c$ decreases the width of the compaction layer decreases as indicated by the behavior of the volume fraction in Figure 23(a) and the compaction rate in Figure 23(b). A shock in the solid phase leads the detonation, which is characteristic of compaction-led structures, and there is a shock in the gas phase near the end of the compaction layer. The shapes of the reaction zone and the drag layer change very little over this range of $\mu_c$, and they simply translate forward in the detonation structure as $\mu_c$ decreases. A similar behavior is seen in the plots of the phase velocities and pressures given in Figure 23(c) and 23(d), respectively.

A further decrease in the compaction viscosity results in a transition from a compaction-led detonation to a reaction-led one. The transition occurs during the time evolution of the solution as indicated in Figure 24. Here, we plot the difference, $\Delta x_{\text{sonic}}(t) = x_{\text{sonic}}(t) - \bar{x}_{\text{sonic}}(t)$, between the position of the leading gas-phase sonic point, $x_{\text{sonic}}(t)$ defined by $|M(x_{\text{sonic}}(t), t)| = 1$, and the position of the leading solid-phase sonic point, $\bar{x}_{\text{sonic}}(t)$ defined by $|M(\bar{x}_{\text{sonic}}(t), t)| = 1$, as a function of time $t$. This difference shows the transition well since compaction-led structures lead with a shock in the solid phase so that $\Delta x_{\text{sonic}}(t) < 0$,
while reaction-led structures lead with a shock in the gas phase so that $\Delta x_{\text{sonic}}(t) > 0$. The early behavior of the piston-driven flows always show a compaction-led structure and a negative difference. For $\mu_c > \mu_c^*$, this structure is maintained and becomes the long-time steady behavior. For smaller values of $\mu_c$, the early compaction-led structure transitions to a reaction-led structure, as indicated in the figure, and the time of transition decreases with decreasing $\mu_c$. The small changes in the solution leading up to transition are delicate and we use a very fine grid with $l_{\text{max}} = 6$ in order to capture the time of transition accurately. It is interesting to note that for $\mu_c < \mu_c^*$, the positive difference between the sonic points is nearly constant, which suggests that the long-time reaction-led structures do not change very much with $\mu_c$ after transition. In fact, we have found this to be the case as we discuss below.

A closer examination of the time-evolution of the solution during transition for the case $\mu_c = 0.01 < \mu_c^*$ is shown in the sequence of plots in Figure 25. The plots focus on the behavior from $t = 18.1$ to 19.1 at intervals of 0.1. For $t < 18.1$, the wave appears to be a steady compaction-led detonation with only subtle indicators of the transition to come. These indicators include a slight decrease in the peak of the solid-phase volume fraction (see Figure 25(a)) and a slight advance of the front of the reaction zone into the tail of the compaction layer (see Figure 25(b)). Upon passage of the reaction zone to the head of the detonation wave, the width of the layer of velocity disequilibrium increases, typical of reaction-led structures, while the layer of pressure disequilibrium all but vanishes, indicative of an approach to the asymptotic behavior for small $\mu_c$ (with $\delta$ fixed).

We find that the steady, reaction-led structures do not change significantly for $\mu_c < \mu_c^*$. For example, the steady structures for $\mu_c = 0.01, 0.005$ and 0.0025 are shown in Figure 26. Here, we observe that the
Figure 22: Steady compaction-led detonation structures for $\sigma = 4$, $\mu_c = 0.05$, $H = 0.2$ and $\delta = 13.5$, 20, 50 and 100. Profiles of (a) volume fractions, (b) rates of reaction, compaction and drag, (c) phase velocities relative to the steady wave and (d) phase pressures $\bar{p} - \beta$ (solid curves) and $p$ (dashed curves). (The reaction rate is scaled by a factor of 5 for illustration purposes.)

volume fraction curves in Figure 26(a) nearly lie on top of one another with only a slight difference occurring at the very front of the structures. This difference is due to a very thin layer of negative compaction, shown in Figure 26(b), which still varies for these small values of $\mu_c$. This small variation has little effect on the reaction rate and drag which appear to have achieved their asymptotic behaviors for small $\mu_c$. The plots of the phase velocities and pressures show little very little change with $\mu_c$ as well, indicating the approach to their respective asymptotic behaviors.

Finally, we consider the effect of varying $\mu_c$ on the early compaction-to-detonation transition time. The results are shown in the $x-t$ plane for three different values of $\mu_c$ in Figure 27. We find that increasing $\mu_c$ slows down the compaction wave, as well as the transition to detonation.

### 7.2.3 Effect of varying $H$

We now discuss briefly the behavior of steady solutions as the heat transfer coefficient $H$ varies. Here we find that the primary change occurs in the profiles of the phase temperatures near the tail of the detonation structure. For example, in Figure 28 we show the temperature of the solid and gas phases for two sets of calculations, one corresponding to the compaction-led structure shown previously in Figure 14 and discussed in Section 7.1.3, and the other corresponding to the reaction-led structure shown previously in Figure 16 and discussed in Section 7.1.4. For both sets, we fix the reaction-rate parameters, $\delta$ and $\mu_c$ to be the same as those used in the previous calculations, but then compute new steady structures for $H = 0.02$, 0.07, 0.2 and 0.5. The solutions within both sets show a peak in the gas temperature, highest in Figure 28(b) for the
Figure 23: Steady compaction-led detonation structures for $\sigma = 4$, $\delta = 15$, $H = 0.2$ and $\mu_c = 0.025$, 0.02 and 0.015. Profiles of (a) volume fractions, (b) rates of reaction, compaction and drag, (c) phase velocities relative to the steady wave and (d) phase pressures $\bar{p} - \beta$ (solid curves) and $p$ (dashed curves). (The reaction rate is scaled by a factor of 5 for illustration purposes.)

Figure 24: Difference in the sonic positions $\Delta x_{\text{sonic}}(t)$ versus time $t$ for $\sigma = 4$, $\delta = 15$, $H = 0.2$ and $\mu_c = 0.005$, 0.01, 0.015 and 0.02. Negative $\Delta x_{\text{sonic}}(t)$ indicates compaction-led detonation structures while positive $\Delta x_{\text{sonic}}(t)$ indicates reaction-led structures.
Figure 25: Transition from compaction-led detonation to reaction-led detonation for \( \sigma = 4 \), \( \delta = 15 \), \( \mu_c = 0.01 \) and \( \mathcal{H} = 0.2 \). Profiles of (a) solid volume fraction, (b) rates of compaction (solid curves) and reaction (dashed curves), (c) velocity of solid (solid curves) and gas (dashed curve) and (d) pressures \( \bar{p} - \beta \) (solid curves) and \( p \) (dashed curves) for \( t = 18.1, 18.2, \ldots, 19.1 \). (The reaction rate is scaled by a factor of 5 for illustration purposes.)

reaction-led detonations, corresponding to the onset of the main reaction zone as discussed previously. The variation in \( \mathcal{H} \) has little effect on this peak and on the general behavior near the front of the detonation structure. The main difference occurs in the solid-phase temperature near the tail of the steady structure. For larger values of \( \mathcal{H} \) we note that the phase temperatures equilibrate more rapidly, but the solid volume fraction is very low in the tail so this change has very little effect on the overall behavior of the steady detonations.

8 Conclusions

A new second-order numerical method, a modification of the standard Godunov scheme for hyperbolic conservation laws, is developed for the Baer-Nunziato model of heterogeneous explosives. The novel feature of the method is the rational manner in which it accommodates, within the Godunov framework, the nozzling terms that appear naturally in the model. This aspect of the method builds upon the early work by the present authors in [14]. The method also employs adaptive mesh refinement, and is thus capable of generating highly resolved and accurate solutions with economy. Previous computational treatments of the model have generally employed substantially lower resolutions, and have included a method-of-lines approach [1, 17], an approach that transforms the governing equations into a parabolic system by introducing a significant diffusive transport [16], or an approach in which the model is modified in such a way that the nozzling terms
Figure 26: Steady reaction-led detonation structure for $\sigma = 4$, $\delta = 15$, $\mathcal{H} = 0.2$ and $\mu_c = 0.01$, 0.005 and 0.0025. Profiles of (a) volume fractions, (b) rates of reaction, compaction and drag, (c) phase velocities relative to the steady wave and (d) phase pressures $\bar{p} - \beta$ (solid curved) and $p$ (dashed curve). (The reaction rate is scaled by a factor of 5 for illustration purposes.)

Figure 27: Wave paths in the $x$-$t$ plane for $\mu_c = 0.05$, 0.025 and 0.01 with $\delta = 15$ and $\mathcal{H} = 0.2$. Dashed curves show the paths of reactionless compaction waves ($\sigma = 0$) while the solid curves show transitions to detonation for $\sigma = 4$ and $p_{ign} = 1.4 \times 10^{-5}$. (Positions are given in the piston frame of reference.)
The study focuses on the steady structure of planar detonations on the one hand, and the evolution to these steady structures on the other. This is done by obtaining solutions to an impact problem over a long time scale, and for a broad range of the problem parameters. The parameters of interest are the prefactor that multiplies the reaction rate, the ignition pressure, the drag coefficient, the compaction viscosity, and to a lesser extent the heat transfer coefficient.

We find that two distinct steady structures emerge, the compaction-led structure and the reaction-led structure. The former is characterized by a lead shock in the solid phase followed by a compaction layer that precedes the main reaction zone, and the latter by a lead shock in the gas phase that is followed immediately by the main zone of reaction. Fixing the remaining parameters we identify, in the plane of the compaction viscosity versus the drag coefficient, a curve of demarcation that separates the two structures. Generally, compaction-led detonations are found for larger rates of drag and smaller rates of compaction, while reaction-led detonations occur otherwise. Changes in structure with variation of parameters across the curve of demarcation are abrupt, but are more gradual in the respective regions on either side of the boundary. A Chapman-Jouguet state can be identified on the fully reacted Hugoniot curve in the plane of mixture pressure and mixture specific volume. Computations show that for either of the two structures, the ultimate steady detonation is slightly faster than the CJ wave, and leads to an end state that is a slight departure from the CJ state on the weak branch of the fully-reacted Hugoniot.

With the steady structures identified, we examine the transient aspects of the reactive impact problem in detail to uncover the reaction-induced processes that result in a transition from the low-speed compaction wave into a high-speed detonation. In the absence of the reaction source term, the result of piston impact is a wave of compaction propagating through the explosive. When the reaction term is included, compaction-induced compression of the gas initiates reaction. Reaction, first initiated at the piston face, converts solid into gas, which moves faster than the solid and attempts to permeate it. Since the depth of permeation is small, the solid serves to confine the gas, thereby raising its pressure. Higher pressure in the gas leads to a higher reaction rate, and the process builds upon itself. Three different processes are available for the exchange of momentum between the gas and the solid: conversion of solid to gas, drag between the phases, and the nozzling effect. In the early stages of evolution drag and nozzling are the principal agents within the reaction zone that transfer momentum from the gas to the solid, thereby accelerating its motion and raising its pressure. As time advances, both nozzling and conversion amplify in magnitude and apply in a broad region of the reaction zone. However, being of opposite signs, these two processes tend to have a small net effect. Drag, on the other hand, continues to dominate, but over a progressively thinner region. Compression of the solid in the reaction zone is carried forward acoustically into the upstream region, and as the reaction strengthens with the passage of time, a shock is generated in each phase. The gas shock serves as the leading edge of the reaction zone, and the solid shock the reaction-driven wavehead. Depending on
the parameters of the model, the shock in the solid phase leading the detonation in its early phase may or
may not be overtaken at a later time by the shock in the gas phase, and this ultimately selects whether the
long-time steady detonation is reaction-led or compaction-led.

To summarize, our study has shown that the speed of an unsupported planar detonation, once established,
is relatively insensitive to the parameters modeling the source terms of the present two-phase model. On the
other hand, the structure of the steady detonation, and the details by which it achieves a steady state, are
highly dependent upon the parameters. Well-resolved numerical calculations are needed to determine these
structures accurately, and solutions have been examined for a wide range of the problem parameters. These
solutions have shed new light on the overall behavior of the two-phase model.

The two-phase formulation has an extensive literature, especially as it pertains to modeling. As such
the model represents a substantial investment, and a careful consideration of both its solution structure
and practical applicability is warranted. The present paper concentrates on the former aspect for relatively
simple constitutive input, but with a sound numerical approach that addresses the nonstandard mathematical
nature of the hyperbolic model. Subsequent to a thorough understanding of solution behavior, comparisons
with experiment can be carried out for more realistic constitutive information.

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