Deformable wall effects on the detonation of combustible gas mixture in a thin-walled tube

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We present a multi-material numerical investigation on the propagation of combustible gas mixture detonation in thin-walled metal tubes. We use experimentally tuned one step Arrhenius chemical reaction and an ideal gas equation of state (EOS) to describe the stoichiometric H₂–O₂ and C₂H₄–O₂ detonations. Purely plastic deformations of copper and stainless steel tubes are modeled by the Mie–Grüneisen EOS and the Johnson–Cook strength model. To precisely track the interface motion between the detonating gas and the deforming wall, we use the hybrid particle level-sets within the ghost fluid framework. The calculated results are compared with the theory and validated against the experimental data. The results on thin-walled tube response explain the process of generation and subsequent interaction of the expansion waves along the tube wall that may further complicate the detonative loading conditions within the tube.

A R T I C L E   A B S T R A C T

Introduction

Detonation wave is a reactive shock wave supported by the rapid chemical reaction that results in a sudden increase of pressure and temperature, leading to an extreme thermodynamic state within a very short time. When it is accompanied by the structural deformation or a failure, such internal explosion and detonation in structures can raise a major safety concern. For instance, the internal explosion of fuel transporting pipe lines may trigger pipe rupture and a catastrophic disaster [1,2]. If one properly understands the mechanism of structure deformation (or failure) induced by the interaction between the gaseous detonation and the confinement structures, aforementioned personnel and material losses by explosion may be minimized.

In recent decades, studies on the detonation and DDT (deflagration to detonation transition) in narrow tubes of varying thickness have been performed by the researchers for building and utilizing the small scale (millimeter size) propulsion and power systems [3–6]. These studies are focused on the internal detonation flow subjected to a rigid boundary wall. When tubes can no longer persist yielding due to a detonative loading, it is then plastically deformed and subsequent response influences the internal flow, likely generating compression or expansion waves. Previously, experimental and numerical studies of deformed or fractured tubes under detonation loading have been conducted [7–11]. These studies accomplished quantitative measurements and numerical predictions of purely elastic or elasto-plastic behaviors of narrow tubes under such loadings.

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Here, we consider in detail the dynamics of a purely plastic response of narrow tubes of varying thicknesses. Despite several reported attempts known to simulate explosively deformed tube due to a condensed phase detonation [12,13], nothing has been done for a purely plastic response of the metal tube subjected to a gas mixture detonation. Thus, the gaseous detonation and its interaction with the thin-walled metal tubes under multi-material treatment are studied, and the obtained results are validated against the experimental data and the theory.

Numerical model

Governing equations

To simulate the dynamic plastic deformation of the tube under detonation loading, the following conservative laws of mass, momentum, energy, chemical species in an axisymmetric cylindrical coordinate are used:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial r} (\rho u_r) + \frac{\partial}{\partial z} (\rho u_z) = 0$$  \hspace{1cm} (1)

$$\frac{\partial (\rho u_r)}{\partial t} + \frac{\partial}{\partial r} (\rho u_r u_r) + \frac{\partial}{\partial z} (\rho u_z u_r) + \frac{\rho u_r^2}{r} - \delta \left( \frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z} \right) = 0$$  \hspace{1cm} (2)

$$\frac{\partial (\rho u_z)}{\partial t} + \frac{\partial}{\partial r} (\rho u_r u_z) + \frac{\partial}{\partial z} (\rho u_z u_z) + \frac{\rho u_z^2}{r} - \delta \left( \frac{\partial \sigma_{rz}}{\partial r} \right) + \frac{\partial \sigma_{zz}}{\partial z} = 0$$  \hspace{1cm} (3)

$$\rho \left( \frac{\partial (\rho Y_i)}{\partial t} + \frac{\partial (\rho Y_i u_r)}{\partial r} + \frac{\partial (\rho Y_i u_z)}{\partial z} \right) - \rho \dot{\phi} = 0$$  \hspace{1cm} (4)

where parameters $\delta = 0$ for reactive gas or $\delta = 1$ for a deformable metal tube. In these equations, $u_r$, $u_z$, $P$, $e$, and $Y_i$ are density, $r$-axis velocity, $z$-axis velocity, pressure, total energy density, chemical energy release and mass fraction of the reactant mixture, respectively. Also $\omega_{\text{tot}}\Delta t / \Delta t_{\text{chem}} = A_B P \exp(-E_0/(RT))$ or the reaction rate is described by the experimentally tuned first-order Arrhenius kinetics which is chosen based on its feasibility to resolve the key characteristics of detonation such as detonation pressure and velocity of propagation. However, any potential weakness associated with using a single step global scheme instead of a detailed mechanism will not be addressed here. By using the adiabatic flame temperature and CJ detonation velocity, the heat capacity ratio, $\gamma$ and chemical energy release, $Q$ are provided. The pre-exponential factor, $A$ and activation energy, $E_A$ are obtained by solving the energy equation of the laminar flame and by using a one-dimensional detonation theory [14]. Within the deformable metal tube, deviatoric stress, $\sigma_{ij}$ fields are calculated together with the evolution equations based on a Hooke's law and the flow theory of plasticity for high strain rate deformation:

$$\frac{\partial \sigma_{rr}}{\partial t} + \frac{\partial (\sigma_{rr} u_r)}{\partial r} + \frac{\partial (\sigma_{rr} u_z)}{\partial z} = 2\tau_{ij} \Omega_{ij} + \tau_{ij} \left( \frac{\partial u_r}{\partial r} + \frac{\partial u_z}{\partial z} \right)$$

$$+ 2G \left( \frac{\partial u_r}{\partial r} - \frac{\partial u_z}{\partial z} \right) - \eta \mathbf{D}_{ij}^p$$  \hspace{1cm} (6)

$$\frac{\partial \sigma_{rz}}{\partial t} + \frac{\partial (\sigma_{rz} u_r)}{\partial r} + \frac{\partial (\sigma_{rz} u_z)}{\partial z} = -2\tau_{ij} \Omega_{ij} + \tau_{ij} \left( \frac{\partial u_r}{\partial r} + \frac{\partial u_z}{\partial z} \right)$$

$$+ 2G \left( \frac{\partial u_r}{\partial r} - \frac{\partial u_z}{\partial z} \right) - \eta \mathbf{D}_{ij}^p$$  \hspace{1cm} (7)

$$\frac{\partial \sigma_{zz}}{\partial t} + \frac{\partial (\sigma_{zz} u_r)}{\partial r} + \frac{\partial (\sigma_{zz} u_z)}{\partial z} = \Omega_{ij} (\tau_{ij} - \tau_{ij}) + \tau_{ij} \left( \frac{\partial u_r}{\partial r} + \frac{\partial u_z}{\partial z} \right)$$

$$+ 2G \left( \frac{\partial u_r}{\partial r} - \frac{\partial u_z}{\partial z} \right) - \eta \mathbf{D}_{ij}^p$$  \hspace{1cm} (8)

here, $\Omega_{ij}$, $G$, $\Sigma$, and $D_{ij}^p$ are spin tensor, shear modulus, volume strain rate, and plastic strain rate tensor, respectively. $\eta$ equals to 0 (or 1) in the elastic (or plastic) state. More in-depth descriptions of the parameters are explained in Ref. [11]. The governing equations are solved by a third-order Runge–Kutta and the ENO (essentially non-oscillatory) method in the temporal and spatial discretization, respectively.

Constitutive relations

The pressure of a combustible gas mixture is calculated by the ideal gas equation of state (EOS), $P = \rho RT/M$. Here, $R$ and $M$ are universal gas constant and molecular weight, respectively. For a description of the deformable metal tube, we use the Mie–Grüneisen EOS and the rate-dependent Johnson–Cook strength model in which the yield stress depends on shear rate and temperature as shown in eqns. (9) and (10) below:

$$p(\rho, e) = \rho_0 \Gamma_0 e \left[ \frac{\rho_0 C_0^2 \phi}{(1 - \phi)^2} \right]$$

$$\frac{1}{2} \Gamma_0 \Gamma_0$$

if $\rho \geq \rho_0$, $\phi = 1 - \frac{\rho_0}{\rho}$

otherwise

$$\sigma_y = \left( a_y C + A (\Gamma^m) \right) \left( 1 + B \ln \left( \frac{\Gamma^m}{\Gamma_{0m}} \right) \right)$$

$$\left( 1 - \frac{T}{T_0} \right)^m$$

(10)

where $\Gamma_0$, $c_0$, $C$, $A$, $B$, $m$ and $\Gamma_{0m}$ are material constants, and $\rho_0$, $T_0$, $T_0$, and $\Gamma_0$ are initial density, melting temperature, ambient temperature, and effective plastic strain rate, respectively. $\phi$ is commonly set to a unity.

Multi-material boundary tracking and treatment

To track the interface between the two different materials such as combustible gas and a metal tube, a hybrid particle level set method is used. For a simple level set equation [12],

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{u} = 0$$  \hspace{1cm} (11)

the interface of each substance can be marked as the points of zero level set ($\phi = 0$). Also, the region with $\phi < 0$ indicates the inner side of the material, and $\phi > 0$ is the region outside the corresponding material. The fifth order Weighted ENO and
third order RK method are used in the spatial and temporal derivatives for Eqn. (11) near the interface (θ = 0). When a rapid change in a material property induces a distortion of the interface during the calculation of the interface level set function, the periodic re-initialization is used to secure the correct solution. In order to avoid these known problems and to obtain the precise interface solution, a hybrid particle level set method is adapted in the present interface tracking [15].

At the interface of two different materials, each material property must jump due to the discontinuous entropy distribution. A ghost fluid method is used to address the aforementioned problem. In this method, ghost cells are distributed on the other side of the material of interest using an extrapolation based on the continuous entropy assumption. Here, the real discontinuity in the entropy merged with the ghost cells generates the proper boundary conditions. Then the same pressure and velocity are imposed in the ghost cells. The entropy in the ghost cells is obtained from the real material. Then the remaining variables are determined from the entropy relation and the equation of state [12].

**Validation of the gaseous detonation model and plastic deformation**

Before performing a fully plastic deformation of the tube subject to an internal detonation, the validations of detonation model, plastic deformation of metal, and multi-material interface tracking are performed. The experimental data of a stoichiometric C2H4–O2 mixture [7] are considered for the comparison.

Fig. 1 shows pressure histories of the experiment and numerical result taken from the four gauges (P1, P2, P3, and P4) which are located at 1764, 1364, 964, and 0 mm from the end wall. The numerical results are based on the parameters of a stoichiometric C2H4–O2 mixture (see Table 1). In this figure, when detonation propagates toward the end wall, the pressure sharpens and the velocity reproduces to its experimental value. Whereas for the reflected shock waves, calculated pressure and velocity are higher than the experimental values. This is mainly due to neglecting the energy loss by friction and heat diffusion as well as turbulent mixing. While the numerical results are fairly descriptive of the measurements of [7], the chemical model is also quite reasonable for depicting the state of detonative internal loading that induces dynamic wall effects.

We further check the residual plastic strain of a 304L stainless steel tube under a detonation loading. In 2D cylindrical coordinate, kinetic mechanism of a stoichiometric C2H4–O2 mixture is used with the Mie–Gruneisen EOS and the rate-dependent Johnson–Cook strength model [17,18] for 304L stainless steel tube. Fig. 2(a) shows the setup, and the mesh size is 0.1 mm. Fig. 2(b) is the comparison of experimental and calculated residual plastic strain using the 2 and 3 bar initial pressure conditions with a plastic strain distribution inside the tube. Here, numerical results are broader than experimental measurements moving away from the wall. This is because the model considers the liquefied solid phase right after the plastic deformation.

**Results and discussion**

We simulated the plastic deformation of an explosively loaded narrow copper tube subject to detonation of a stoichiometric H2–O2 mixture. The considered tube thicknesses are 0.12 and 0.16 mm for ‘deformable’ tube while 0.2 mm thick tube represents a ‘rigid’ tube. All tubes have the same inner radius $r_i = 2$ mm.

**Setup**

We consider a stoichiometric H2–O2 mixture that fills a copper tube having the different thicknesses subjected to a detonation loading. Table 1 shows the initial conditions and the mechanical and chemical parameters of the mixture. Table 2 summarizes the initial parameters of copper. The Mie–Gruneisen EOS and Johnson–Cook strength model are validated by reproducing the Taylor impact result [19] where the maximum radius and residual length are calculated as

**Table 1 – Initial parameters of stoichiometric C2H4–O2 mixture and stoichiometric H2–O2 mixture.**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Stoichiometric C2H4–O2 mixture</th>
<th>Stoichiometric H2–O2 mixture [16]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial density, $p_0$</td>
<td>1.268 kg/m$^3$</td>
<td>0.493 kg/m$^3$</td>
</tr>
<tr>
<td>Initial pressure, $P_0$</td>
<td>$1.003 \times 10^5$ Pa</td>
<td>$1.01 \times 10^5$ Pa</td>
</tr>
<tr>
<td>Initial temperature, $T_0$</td>
<td>295 K</td>
<td>293 K</td>
</tr>
<tr>
<td>Specific heat ratio, $\gamma$</td>
<td>1.232</td>
<td>1.333</td>
</tr>
<tr>
<td>Molecular weight, $M_w$</td>
<td>0.051 kg/mol</td>
<td>0.011853 kg/mol</td>
</tr>
<tr>
<td>Pre-exponential factor, $A_0$</td>
<td>$8 \times 10^8$ m$^{-3}/$(kg s)</td>
<td>$7 \times 10^8$ m$^{-3}/$(kg s)</td>
</tr>
<tr>
<td>Activation energy, $E_a$</td>
<td>59,035 J/mol</td>
<td>69,036 J/mol</td>
</tr>
<tr>
<td>Chemical heat release, $q$</td>
<td>$4.597 \times 10^8$ J/kg</td>
<td>$4.867 \times 10^8$ J/kg</td>
</tr>
<tr>
<td>CJ detonation pressure</td>
<td>$3.26 \times 10^8$ Pa</td>
<td>$1.773 \times 10^8$ Pa</td>
</tr>
<tr>
<td>CJ detonation velocity</td>
<td>2943 m/s</td>
<td>2845 m/s</td>
</tr>
</tbody>
</table>
7.29 mm and 21.53 mm while the experimental values are 7.27 mm and 21.4 mm, respectively.

In order to fulfill the mesh resolution requirement, we first consider a 1D detonation calculation by varying the mesh size. Fig. 3 shows pressure profiles of four different mesh sizes 0.1, 0.05, 0.02, and 0.01 mm in detonations of a stoichiometric H₂–O₂ mixture. Here, 0.02 and 0.01 mm resolutions show an identical detonation structure in terms of its position and strength of a von Neumann spike and CJ pressure. Accordingly, we use 0.02 mm resolution which is reasonable to reproduce the pressure and detonation velocity, although the mesh size is coarser than those used by Ref. [20]. Fig. 4(a) shows pressure profiles of stoichiometric H₂–O₂ mixture model for various initial pressures. In this figure, CJ pressure is proportional to the initial pressure in both numerical and experimental data [21]. Fig. 4(b) shows profiles of pressure, species, reaction rate and temperature near detonation front in a stoichiometric H₂–O₂ mixture under initial pressure, 0.101 MPa. Here, the peak pressure, CJ pressure, and CJ temperature are 3.38 MPa, 1.89 MPa and 3060 K, respectively, all of which are in good agreement with the experimental data.

The 2D cylindrical domain is shown in Fig. 5, where section of a detonation tube (r₁ = 2 mm; L = 20 mm) is considered with the three different tube thicknesses. The boundary conditions of top, left, right, and bottom are wall, symmetric, zero gradient, and extrapolated conditions (X_{boundary} = 0.95X₁ + 0.05X₀), respectively. For detonation initiation, a CJ condition is initially assigned near the bottom.

**Rigid tube (0.2 mm thickness tube)**

We simulate the detonation in a narrow tube of 2 mm inner radius and 0.2 mm thickness as a rigid tube. Fig. 6 shows the

### Table 2 – Initial parameters of copper tube.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Copper [11]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial density, ρ₀</td>
<td>8930 kg/m³</td>
</tr>
<tr>
<td>Initial temperature, T₀</td>
<td>293 K</td>
</tr>
<tr>
<td>Shear modulus, G</td>
<td>43.33 GPa</td>
</tr>
<tr>
<td>Poisson’s ratio, ν</td>
<td>0.35</td>
</tr>
<tr>
<td>Heat capacity, c</td>
<td>383.5 W/(m K)</td>
</tr>
<tr>
<td>Gruneisen coefficient, Γ₀</td>
<td>2.0</td>
</tr>
<tr>
<td>Normal sound speed, c₀</td>
<td>3940 m/s</td>
</tr>
<tr>
<td>s</td>
<td>1.49</td>
</tr>
<tr>
<td>Initial yield strength, σ_{Y₀}</td>
<td>90 MPa</td>
</tr>
<tr>
<td>A</td>
<td>292 MPa</td>
</tr>
<tr>
<td>n</td>
<td>0.31</td>
</tr>
<tr>
<td>B</td>
<td>0.025</td>
</tr>
<tr>
<td>m</td>
<td>1.09</td>
</tr>
</tbody>
</table>

![Fig. 3 – Pressure profiles of four different mesh sizes (0.1, 0.05, 0.02, and 0.01 mm).](image)

![Fig. 2 – (a) Schematic of a 2D simulation setup. (b) Comparisons of experimental and numerical results of residual plastic strain.](image)
snapshots of evolving density field. Here, the detonation propagates from the bottom with a velocity 2844 m/s. Then the reflected shock wave propagates from the top with a velocity 2000 m/s (see Fig. 6(c)).

Fig. 7 shows the pressure profiles in 1D and 2D cylindrical coordinates. The velocities of detonation and reflected shock wave in 2D are identical to 1D ideal model. In the presence of a perturbation at the flame front by the thermal instability of detonation, however, complex unstable structure develops in the propagation direction, as the maximum pressure fluctuates and the pressure becomes higher than the von Neumann spike (3.38 MPa) of a plane detonation. Here we can also find out that the detonation velocity, CJ pressure, and maximum reflected shock wave pressure are 2844 m/s, 1.89 MPa, and 5 MPa ($P_{ref}/P_{CJ} = 2.6$), respectively.

**Thin-walled tube (0.12 and 0.16 mm thickness tube)**

Contrary to the rigid tube result, the thin-walled tube is a deformable one under the high pressure loading by a detonation pressure. The thin tubes of 2 mm inner radius and 0.12 and 0.16 mm thickness are subjected to the same intensity of the aforementioned detonation loadings.

Before discussing the numerical study on plastic deformation of the thin-walled tube, a theoretical model [22–24] is considered, which states the dynamic amplification factor (DAF), $\Phi$ and the critical burst pressure, $P_{brust}$ for plastic
displacement in the thin-walled tube under detonation loading. DAF is a ratio between the maximum dynamic strain $\varepsilon_{\text{dynamic,max}}$ and the static strain $\varepsilon_{\text{static}}$ based on [22].

$$\Phi(v) = \frac{\varepsilon_{\text{dynamic,max}}(v)}{\varepsilon_{\text{static}}} = \frac{w_{\text{max}}(v)}{w_{v=0}} \tag{12}$$

Three different thicknesses (0.12, 0.16, and 102 mm) of copper tube are considered whose parameters are listed in Table 2. In Fig. 8, DAF of 2.3 and 2.04 are obtained at detonation velocity of 2844 m/s and reflected shock velocity of 2000 m/s for $\text{H}_2-\text{O}_2$ mixture, respectively.

Table 3 - Theoretical burst pressure under detonation and reflected waves.

<table>
<thead>
<tr>
<th>Tube thickness (mm)</th>
<th>Detonation 2844 m/s (MPa)</th>
<th>Reflected shock 2000 m/s (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.12</td>
<td>2.22</td>
<td>2.57</td>
</tr>
<tr>
<td>0.16</td>
<td>2.93</td>
<td>3.39</td>
</tr>
<tr>
<td>0.2</td>
<td>3.64</td>
<td>4.2</td>
</tr>
</tbody>
</table>

As for the thin-walled copper tube, we check the burst pressure given by a simple expression from Ref. [24]:

$$p_{\text{burst}} \approx \sigma_Y \frac{t}{\Phi(r_i + t/2)} \tag{13}$$

The equation gives an approximation to a critical pressure upon onset of plastic deformation. The pressure is determined by inner radius $r_i$, thickness $t$, yield stress $\sigma_Y$ of the tube ($\sim 90$ MPa), and $\Phi = 2.3$ and 2.04. Table 3 shows burst pressure under detonation and reflected shock conditions for different tube thicknesses. The pressures of detonation and reflected shock are roughly 2 and 3 MPa, respectively (see Fig. 7). Therefore one can expect that 0.12 mm and 0.16 mm tubes will deform under these conditions. In contrast, the 0.2 mm thickness tube behaves as if a rigid tube having a zero deformation.

Fig. 9 shows the density field of a 0.12 mm thickness tube. When the effective plastic stress exceeds the tube yield stress,
the tube expands outwards and the expansion waves propagate toward the combustible gas (see Fig. 9(b) and (c)). The expansion wave pressure is approximately 0.9 times the ambient detonation pressure. As the tube expands, multiple expansion waves are generated in the contact surface between the gas and the tube, as more complex flow field is constructed by the wave interactions. As a result, pressures and densities are decreased near the bottom side as compared to the rigid tube results.

For the case of a 2 mm inner radius and 0.16 mm thick narrow tube under detonation loading, a direct deformation does not occur; instead, the reflected shock wave whose maximum pressure (~5 MPa, $P_{ref}/P_{CJ} = 2.6$) is higher than detonation pressure causes the tube to respond. Fig. 10 shows snapshots of a density field in a 0.16 mm thickness narrow tube. Before deformation occurs by reflected shock waves, the flow field is identical to a rigid tube case. Once the reflected shock waves are generated and propagated, a sudden change in the flow field and the tube deformation occur (see Fig. 10(b) and (c)). Near the top, the expansion of tube begins and multiple expansion waves are generated in the contact surface as similarly done in the bottom of a 0.12 mm thickness tube.

To confirm deformable wall effects such as the generation and superposition of the expansion waves, we performed simulation of tube deformation for different tube thicknesses under the same inner radius and detonation loading conditions. First, we compare the thin-walled tube of 0.12 mm thickness tube against a rigid tube. In Fig. 11, flames propagate at the same velocity in both thin-walled and rigid tubes. The properties of the product gas are however noticeably changed upon tube deformation. The pressure of a rigid tube is approximately 0.4 MPa near the bottom at all times. However, in the case of the thin-walled tube with time, the pressure and density were decreased due to multiple generations of the expansion waves due to tube deformation that shows the increase of effective plastic strain (see Fig. 11(b) and (c)).
decreasing pressure and density were discovered even in the case of 0.16 mm case. In Fig. 12(a), the pressure decreases near the top as opposed to the uniform pressure in the bottom, even when reflected shock velocity is unchanged. Also the density field in the thin-walled tube showed that the lower density (approximately 0.9 times the ambient density) is localized near the top by deformation (see Fig. 12(b) and (c)).

Conclusion
A careful evaluation of the wall boundary response to explosively loaded conditions and purely plastic deformation of metal tubes is performed in the context of multi-material high-strain rate phenomena involving detonative gas mixtures and their strong interaction with the metal tubes. Using the theory on DAF and burst pressure, the plastic response of a copper tube of three different thickness (0.12, 0.16, and 0.2 mm) having the inner radius of 2 mm is considered under the stoichiometric $\text{H}_2 - \text{O}_2$ detonation loading. The numerical simulation of the tube response under the same loading conditions confirms the results being consistent with the pipe failure theory. The key feature of the present numerical formulation is in the multi-material shock physics technique that solves the instantaneous response of both solid (tube) as well as fluid (detonation loaded complex internal flow) at a high-order accuracy. Thus the results reported here may provide new insight into understanding the overall safety of a gas pipe system consisting of thin-walled metal tubes.

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