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

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ABSTRACT

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 H_2–O_2 and C_2H_4–O_2 detonations. Purely plastic deformations of copper and stainless steel tubes are modeled by the Mie–Gruneisen 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.

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:

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

$$\frac{\partial}{\partial t}(\rho u_r)+\frac{\partial}{\partial r}\left(\rho u_r^2+P\right)+\frac{\partial}{\partial z}(\rho u_r u_z)+\frac{\rho u_r^2}{r} - \delta\left(\frac{\partial \tau_{rr}}{\partial r}+\frac{\partial \tau_{rz}}{\partial z}+\frac{2\tau_{rr}+\tau_{zz}}{r}\right)=0 \tag{2}$$

$$\frac{\partial}{\partial t}(\rho u_z)+\frac{\partial}{\partial r}(\rho u_r u_z)+\frac{\partial}{\partial z}\left(\rho u_z^2+P\right)+\frac{\rho u_r u_z}{r}-\delta\left(\frac{\tau_{rz}}{r}+\frac{\partial \tau_{rz}}{\partial r}+\frac{\partial \tau_{zz}}{\partial z}\right)=0 \tag{3}$$

$$\frac{\partial}{\partial t}(\rho e)+\frac{\partial}{\partial r}\{u_r(\rho e+P)\}+\frac{\partial}{\partial z}\{u_z(\rho e+P)\}+\frac{u_r(\rho e+p)}{r}-\varphi\rho Q\dot{w} - \delta\left\{\frac{u_r\tau_{rr}+u_z\tau_{rz}}{r}+\frac{\partial(u_r\tau_{rr}+u_z\tau_{rz})}{\partial r}+\frac{\partial(u_r\tau_{zr}+u_z\tau_{zz})}{\partial z}\right\}=0 \tag{4}$$

$$\varphi\left\{\frac{\partial}{\partial t}(\rho Y_i)+\frac{\partial}{\partial r}(\rho Y_i u_r)+\frac{\partial}{\partial z}(\rho Y_i u_z)-\rho\dot{w}\right\}=0 \tag{5}$$

where parameters $\varphi=0$ (and $\delta=1$) for reactive gas or $\varphi=1$ (and $\delta=0$) for a deformable metal tube. In these equations ρ, u_r, u_z, P, e, Q, 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 $\dot{w}\equiv\partial Y_i/\partial t|_{Chem}=A\rho Y\exp(-E_a/(RT))$ 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, γ 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, τ_{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:

$$\frac{\partial \tau_{rr}}{\partial t}+\frac{\partial(\tau_{rr}u_r)}{\partial r}+\frac{\partial(\tau_{rr}u_z)}{\partial z}=2\tau_{rz}\Omega_{rz}+\tau_{rr}\left(\frac{\partial u_r}{\partial r}+\frac{\partial u_z}{\partial z}\right) +2G\left(\frac{\partial u_r}{\partial r}-\sum-\eta D_{rr}^{p}\right) \tag{6}$$

$$\frac{\partial \tau_{zz}}{\partial t}+\frac{\partial(\tau_{zz}u_r)}{\partial r}+\frac{\partial(\tau_{zz}u_z)}{\partial z}=-2\tau_{rz}\Omega_{rz}+\tau_{zz}\left(\frac{\partial u_r}{\partial r}+\frac{\partial u_z}{\partial z}\right) +2G\left(\frac{\partial u_z}{\partial z}-\sum-\eta D_{zz}^{p}\right) \tag{7}$$

$$\frac{\partial \tau_{rz}}{\partial t}+\frac{\partial(\tau_{rz}u_r)}{\partial r}+\frac{\partial(\tau_{rz}u_z)}{\partial z}=\Omega_{rz}(\tau_{zz}-\tau_{rr})+\tau_{rz}\left(\frac{\partial u_r}{\partial r}+\frac{\partial u_z}{\partial z}\right) +2G\left(\frac{1}{2}\left(\frac{\partial u_r}{\partial z}+\frac{\partial u_z}{\partial r}\right)-\eta D_{rr}^{p}\right) \tag{8}$$

here, Ω_{ij}, G, Σ, and D_{ij}^{p} are spin tensor, shear modulus, volume strain rate, and plastic strain rate tensor, respectively. η 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–Gruneisen 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:

$$p(\rho,e)=\rho_0\Gamma_0 e+\begin{cases}\dfrac{\rho_0 c_0^2\varphi}{(1-s\varphi)^2}\left[1-\dfrac{\Gamma_0}{2}\varphi\right] & \text{if } \rho\ge\rho_0 \\ c_0^2(\rho-\rho_0) & \text{otherwise}\end{cases},\quad \varphi=1-\frac{\rho_0}{\rho} \tag{9}$$

$$\sigma_Y=\left(\sigma_{Y,0}+A\left(\bar{\varepsilon}^{P}\right)^{n}\right)\left(1+B\ln\left(\frac{\dot{\bar{\varepsilon}}^{P}}{\dot{\varepsilon}_0}\right)\right)\left(1-\left(\frac{T-T_0}{T_m-T_0}\right)^{m}\right) \tag{10}$$

where Γ_0, s, c_0, A, B, n are material constants, and ρ_0, T_m, T_0, and $\dot{\bar{\varepsilon}}^{P}$ are initial density, melting temperature, ambient temperature, and effective plastic strain rate, respectively. $\dot{\varepsilon}_0$ 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],

$$\frac{\partial \phi}{\partial t}+\vec{V}\cdot\nabla\phi=0 \tag{11}$$

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