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Structure and flame speed of dilute and dense layered coal-dust explosions

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Multidimensional time-dependent simulations were performed to study the interaction of a stoichiometric methane–air detonation with layers of coal dust. The simulations solved equations representing a Eulerian kinetic-theory-based granular multiphase model applicable to dense and dilute particle volume fractions. These equations were solved using a high-order Godunov-based method for compressible fluid dynamics. Two dust layer concentrations were considered: loose with an initial volume fraction of 1%, and dense with an initial volume fraction of 47%. Each layer was simulated with two types of dust: reactive coal and inert ash. Burning of the coal particles results in a coupled complex consisting of an accelerating shock leading a coal-dust flame. The overall structure of the shock–flame complex resembles that of a premixed fast flame with length scales on the order of several meters. The large length scales are direct results of time needed to lift, mix, heat, and autoignite the particle. The flame speeds are large and much larger than the gas-phase velocity. Large spikes of flame speed are characteristic of the 47% case. These spikes and high flame speed are caused by pockets of coal dust autoigniting ahead of the flame. The flame is choked in the 1% case due to the gas-phase products exceeding the sonic velocity with respect to the flame. The 47% case is choked due to attenuation of pressure waves as they propagate through particles. Inert layers of dust substantially reduce the overpressure, impulse, and speed produced by propagating blast wave. The results also show that loose layers of dust are far more dangerous than dense layers. The shock and flame are more strongly coupled for loose layers, propagate at higher velocity, and produce large overpressures and impulses.

1. Introduction

Dust explosions have been significant hazards for centuries in the process and mining industries where layers of dust can accumulate. These layers are usually unreactive in bulk form, but can react violently when turbulent post-shock flow, induced by a primary explosion, disperses the particles. The aerosolized dust then ignites and produces pressure waves that interact with and accelerate the lead shock (Houim and Oran, 2015; Semenov et al., 2013). Combustion of lifted and aerosolized dust can produce pressures over 10 bar, propagate at speeds over of 1000 m/s, and possibly transition to detonation (Houim and Oran, 2015; Li et al., 1995a; Semenov et al., 2013).

Modeling of layered dust explosions ranges from phenomenological (Edwards and Ford, 1988) to industrial codes that use empirical dust lifting and other correlations to simulate large-scale explosions (Skjold et al., 2007). Relatively few studies have attempted to model layered dust explosions without the use of these correlations (Houim and Oran, 2015; Semenov et al., 2013) by resolving the dust layer and treating it as a granular and porous material that can move. Analysis of the detailed flame structure of a layered coal dust explosion was recently performed by Houim and Oran (2015). The structure of a layered coal dust explosion consists of a shock–flame complex (SFC), which is a shock leading a turbulent, nonpremixed coal dust flame. Burning of the coal dust is mainly from carbon char that mixes with air by relative velocity between the gas and solid phases. Reactions of volatized methane are of secondary importance to the dynamics of the SFC. The SFC propagates at much faster speeds than can be explained by the local laminar flame speed of lifted coal dust. The high flame velocity was found to be caused by an autoignition wave of burning coal dust.

This paper presents simulations of a blast wave produced from a methane detonation interacting with a thin layer of reactive coal dust and inert ash in a thin channel. We model the solid particles

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using kinetic theory-based multiphase flow equations (Gidsapow, 1994), which accounts for particle–particle interactions and is valid for particle volume fractions, α_s, ranging from dilute to near the packing limit. Two different dust layer concentrations are considered: α_s of 47% (Edwards and Ford, 1988) and 1%, which is comparable to that described by Semenov et al. (2013). The resulting coal bulk densities inside the layers for the two cases were 564 kg/m^3 and 12 kg/m^3. The average coal bulk density, if dust uniformly filled the channel, would be 0.48 kg/m^3 and 22 kg/m^3 for the dilute and dense cases, respectively. The 17 coupled governing partial differential equations were solved using a recently developed high-order Godunov-based numerical method (Houim and Oran, 2013).

Our previous paper (Houim and Oran, 2015) focused on the structure of the flame and ignition mechanism of the shock–flame complex. In this paper we focus on the overall structure of the shock–flame complex, the flame velocity relative to the shock, and the effect of an inert dust layer on attenuating the shock resulting from the failure of a gaseous methane–air detonation.

2. Physical and numerical model

Fig. 1 shows the initial and boundary conditions for the simulations. The domain is 20 m long. The bottom 2 mm contain a layer of coal dust or ash. The first two meters of the domain contain a stoichiometric mixture of methane and air at 1 bar and 300 K. The remaining 18 m is transitioned to pure air over a distance of 0.4 m by a hyperbolic tangent function. Initially, two large hot pockets of unreacted fuel and air (at 10 bar and 1000 K) trigger a detonation.

The coal dust has a diameter of 30 μm, a specific heat of 987 J/kg K, and a material density, ρ_s, of 1200 kg/m^3. The dust was assumed to be brown coal with initial mass fractions of carbon and CH_4 of 39.1% and 54.5%, respectively (Semenov et al., 2013). The inert dust was 100% ash.

2.1. Governing equations

Seven gas-phase species are considered: $O_{2,g}$, $CO_{2,g}$, CO_g, O_g, $CH_{4,g}$, H_2O_g, and $N_{2,g}$. The granular phase consists of three species within each coal particle: volatiles ($CH_{4,s}$), carbon char (C_s), and ash. Subscripts g and s refer to the gas and solid phases, respectively. Effects from radiation energy transport, heat conduction, mass diffusion, and viscous stresses are neglected. Justification of these assumptions is discussed in Houim and Oran (2015). The governing equations can be summarized as

$$\frac{\partial \alpha_g \rho_g Y_{g,i}}{\partial t} + \nabla\cdot \alpha_g \rho_g Y_{g,i} \mathbf{v}_g = \alpha_g \dot{\omega}_{g,i} + \dot{m}_{g,i} \quad (1)$$

$$\frac{\partial \alpha_g \rho_g \mathbf{v}_g}{\partial t} + \nabla\cdot\left(\alpha_g \rho_g \mathbf{v}_g \mathbf{v}_g\right) = -\alpha_g \nabla p_g - \mathbf{f}_{\text{Drag}} - \mathbf{f}_{\text{Lift}} + \mathbf{v}_s \dot{M} \quad (2)$$

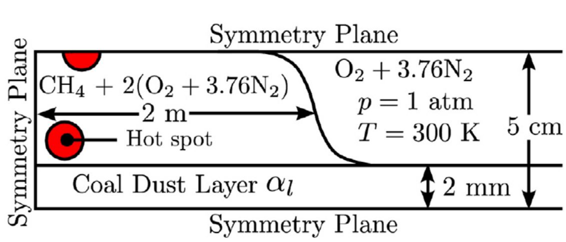

Fig. 1. Initial and boundary conditions for the two-dimensional simulations (Houim and Oran, 2015).

$$\frac{\partial \alpha_g \rho_g E_g}{\partial t} + \nabla\cdot\left[\alpha_g \mathbf{v}_g \left(\rho_g E_g + p_g\right)\right] = -p_g \nabla\cdot(\alpha_s \mathbf{v}_s) - q_{\text{conv}} + \phi_{\text{visc}} - \left(\mathbf{f}_{\text{Drag}} + \mathbf{f}_{\text{Lift}}\right)\cdot\mathbf{v}_s - \phi_{\text{slip}} + e_s \dot{M} \quad (3)$$

$$\frac{\partial \alpha_s \rho_s}{\partial t} + \nabla\cdot(\alpha_s \rho_s \mathbf{v}_s) = -\dot{M} \quad (4)$$

$$\frac{\partial \alpha_s \rho_s Y_{s,i}}{\partial t} + \nabla\cdot\left(\alpha_s \rho_s Y_{s,i} \mathbf{v}_s\right) = \dot{m}_{s,i} \quad (5)$$

$$\frac{\partial \alpha_s \rho_s \mathbf{v}_s}{\partial t} + \nabla\cdot(\alpha_s \rho_s \mathbf{v}_s \mathbf{v}_s) + \nabla p_s + \nabla p_{\text{fric}} = -\alpha_s \nabla p_g + \mathbf{f}_{\text{Drag}} + \mathbf{f}_{\text{Lift}} - \mathbf{v}_s \dot{M} \quad (6)$$

$$\frac{\partial \alpha_s \rho_s E_s}{\partial t} + \nabla\cdot(\alpha_s \rho_s E_s \mathbf{v}_s) = -p_s \nabla\cdot\mathbf{v}_s - \dot{\gamma} - \phi_{\text{visc}} + \phi_{\text{slip}} - E_s \dot{M} \quad (7)$$

$$\frac{\partial \alpha_s \rho_s e_s}{\partial t} + \nabla\cdot(\alpha_s \rho_s e_s \mathbf{v}_s) = q_{\text{conv}} - e_s \dot{M} + \dot{\gamma}, \quad (8)$$

where α_g, $Y_{g,i}$, ρ_g, p_g, T_g, E_g, $\mathbf{v}_g$ represent the volume fraction, mass fraction of species i, density, pressure, temperature, total energy, and velocity components for the gas phase, respectively. α_s, $Y_{s,i}$, ρ_s, T_s, $\mathbf{v}_s$ are the volume fraction, mass fraction of species i, density, and temperature for the solid phase, respectively. p_s, p_{fric}, e_s, E_s, and $\dot{\gamma}$ are the solids pressure, frictional-collisional pressure, internal energy, pseudo-thermal energy from random translational kinetic energy, and dissipation of E_s from inelastic particle collisions. The homogeneous reaction rate due to chemical reactions is denoted by $\dot{\omega}_i$. The net rate of phase change from the granular to the gas-phase is represented by $\dot{M}$ and the mass production rate of species i due to phase change is denoted by $\dot{m}_{g,i}$. The interphase exchange terms $\mathbf{f}_{\text{Drag}}$, $\mathbf{f}_{\text{Lift}}$, and q_{conv} are the forces due to drag and lift, and convective heat transfer. Dissipation of random granular kinetic energy due to gas-phase viscosity and production due to gas-particle slip are denoted by ϕ_{visc} and ϕ_{slip}, respectively.

The ideal-gas equation-of-state is used for the gas phase. The solids pressure, p_s, is (Gidsapow, 1994),

$$p_s = \rho_s \Theta[\alpha_s(1 + 2(1+e)\alpha_s g_0)], \quad (9)$$

where e is the coefficient of restitution, which assumed to be a constant of 0.99. The granular temperature, Θ, is defined by

$$\Theta = \frac{2}{3}\frac{E_s}{\alpha_s \rho_s}. \quad (10)$$

The radial distribution function, g_0, is defined by (Gidsapow, 1994),

$$\frac{1}{g_0} = 1 - \left(\frac{\alpha_s}{\alpha_{s,\max}}\right)^{1/3}, \quad (11)$$

where $\alpha_{s,\max}$ is the packing limit with a value of 0.65. Frictional-collisional pressure is used in highly packed granular regions (Johnson and Jackson, 1987),

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