

Modeling and Numerical Simulation of Layered Coal-Dust Explosions behind a Propagating Shock Wave

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1 Introduction

Dust lifting behind shock waves is a process that is especially interesting for engineers and researchers dealing with safety problems connected with dust explosions. When a shock wave propagates over a dust layer composed of dust particles, the particles are lifted and dispersed, leading to a dust cloud in the shock induced flow. This phenomenon often occurs in tunnels of coal mine or ducts of facility, and is serious industry issue. Lifting particles have very high combustion velocity because more dispersed particle acquires more oxygen, which is necessary for combustion. Consequently, this larger dust cloud in the presence of an ignition source cloud creates a severe dust explosion. The problems of lifting and dispersing of a dust layer behind a propagating shock wave must therefore be understood to ensure safety regarding dust explosion hazards. In addition, this problem has been contributed by many researchers in terms of collisions of particles and a curvature of the shock wave due to interference between fluid and particles.

Although some works have investigated the dust lifting phenomena, few consider the combustion characteristics behind propagating shock wave, which can hardly be obtained experimentally. Recently, numerical analysis of the structure of a layered coal dust explosion was performed based on Euler-Euler approach, which treats particle phase as continuous phase. The purpose of this study is therefore to investigate the initial process of the layered coal-dust explosions behind a propagating shock wave by using numerical simulation based on Euler-Lagrange approach. Two cases were considered: a dilute oxygen flow with an initial concentration of 24%, and a dense oxygen flow with an initial concentration of 50%.

2 Description of model

2.1 Computational domain and conditions

The geometry of the shock tube for coal dust combustion is shown schematically in Fig. 1. It consists of a rectangular duct of 50 mm in height with a ditch of 80 mm (length) x 2 mm (depth) containing the coal particles of 100 μm in diameter. The coal dust has a density of 980 kg/m^3 . The dust was assumed to be brown coal with initial mass fraction of coal char and methane of 39.1% and 54.5 %, respectively. Air at a temperature of 294 K and standard atmospheric pressure is filled in the duct. For the boundaries of upper and lower wall, slip boundary conditions were used. The 0th-order extrapolations were used for boundaries of the inlet and outlet boundaries of the computational domain.

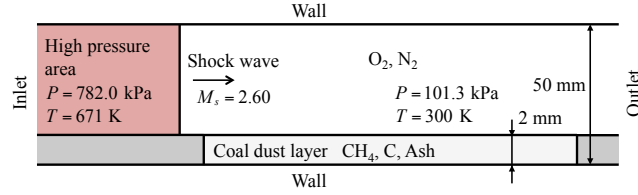


Figure 1. Initial and boundary conditions for a layered coal-dust combustion system.

2.2 Governing equations for the gas phase

The model equations used in the simulation of this work are outlined. The gas phase is treated as a continuous phase in the two-fluid model and described via the Euler equations, modified to include the fluid volume fraction as well as the gas-particle interaction due to the drag force. Accordingly, the conservation of mass, momentum, energy and masses of components for the gas phase are

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g) = \frac{d}{dt}(m_v + m_c) \quad (1)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g \mathbf{u}_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g \mathbf{u}_g) = -\alpha_g \nabla p_g - \mathbf{f}_p + \frac{d}{dt}(m_v + m_c) \mathbf{u}_p \quad (2)$$

$$\frac{\partial}{\partial t}(\alpha_g e_g) + \nabla \cdot \{\alpha_g (e_g + p_g) \mathbf{u}_g\} = \mathbf{f}_p \cdot \mathbf{u}_p + \frac{dm_g}{dt} \cdot q_g + \frac{d}{dt}(m_v + m_c) \left(\frac{\mathbf{u}_p \cdot \mathbf{u}_p}{2} \right) - n_p q_p \quad (3)$$

and

$$\frac{\partial}{\partial t}(\alpha_g \rho_g Y_k) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g Y_k) = \frac{dm_k}{dt} \quad (4)$$

where α_g , ρ_g , $\mathbf{u}_g$, p_g , and e_g are the gas volume fraction, density, velocity, pressure, and energy, respectively. $\mathbf{u}_p$ is particle velocity. Y_k , and m_k denote the mass fraction and mass of species k , and m_v and m_c represent the volatile and coal mass released from the coal, respectively. m_g is the gaseous methane mass, q_g is heat gain due to the methane gas combustion, $\mathbf{f}_p$ is the force acting on the solid particles, n_p is the number density of the particles, and q_p is the heat flux defined by $q_p = h(T_g - T_p)$, where h , T_g , and T_p are the heat transfer coefficient and gas and particle temperature, respectively. The ideal gas equation of state is used to relate pressure, chemical composition, temperature, and density of the gas phase,

$$p_g = \rho_p R T_g \sum_k \frac{Y_k}{M_k} \quad (5)$$

where R is the universal gas constant, M_k is the molecular weight of species k .

2.3 Governing equations for the particle phase

The equation of motion for the representative coal particles is given by

$$\frac{\partial}{\partial t}(\alpha_p \rho_p \mathbf{u}_p) + \nabla \cdot (\alpha_p \rho_p \mathbf{u}_p \mathbf{u}_p) = -\alpha_p \nabla p_g + \mathbf{f}_p - \mathbf{f}_i - \frac{d}{dt}(m_v + m_c) \mathbf{u}_p - \alpha_p \rho_p \mathbf{g} \quad (6)$$

where α_p is the solid volume fraction, which was calculated as $\alpha_p = 1 - \alpha_g$, ρ_p is the solid density, $\mathbf{f}_i$ is the inter-particle force, $\mathbf{g}$ is the specific gravity force. Note that in the above interphase force the drag force [1] and Magnus force [2] are considered. However, the added mass effects and Basset history force have been neglected, because they play a minor role for the type of flows considered here, where the gas density is negligible as against the solid density [3]. The details of the inter-particle

forces are given below. The particle temperature T_p was calculated by considering the heat transfer due to convection and heat gain due to char combustion, using the following equation.

$$m_p c_p \frac{dT_p}{dt} = h S_p (T_g - T_p) - q_c \frac{dm_c}{dt} \quad (7)$$

where c_p , S_p , and q_c are the particle specific heat, surface area, and heat gain due to the char combustion. The particle to particle collisions are modeled by the isotropic solids stress τ . The solids stress derived from the solid volume fraction α_p , which is mapped on the grid. The solids stress model used here is the form proposed by Andrews [4] and is expressed as follows.

$$f_i = \nabla \tau \quad (8)$$

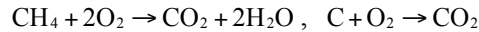
and

$$\tau = P_p \frac{\alpha_p^\beta}{\max[(\alpha_{cp} - \alpha_p), \varepsilon(1 - \alpha_p)]} \quad (9)$$

where P_p is a constant with unit of pressure, β is also a constant, α_{cp} is a solid volume fraction at maximum packing, ε is a small number to remove the peculiarity. The values assigned to P_p , β , and α_{cp} are similar to those employed by Patanker *et al.* [5] and are 100 Pa, 3, and 0.6, respectively.

2.4 Chemical reaction rate model

Gaseous methane combustion and coal char combustion were calculated. The chemical mechanism consists of two global reactions.



Coal devolatilization was simulated by a first-order single reaction model proposed by Badzioch *et al.* [6]. The rates of mass consumption for reactants CH_4 is given as an Arrhenius expression. The values of kinetic parameters, namely, the pre-exponential factor and activation energy are taken from Beak *et al.* [7]. The char burning rate were calculated using Field's model [8].

2.5 Computational method

The discretization method of convection term was simple high-resolution upwind scheme (SHUS) [9]. Third-order space accuracy was obtained using monotonic upwind scheme for conservation laws for the primitive variable interpolation. The time integral method was the 2-step Runge-Kutta method. The minimum cell size was 0.10 mm, and the cells near the dust layer were refined.

3 Results and discussion

The computed time sequences of gas phase temperature for the dilute oxygen case are shown in Fig. 2. The shock wave at 0.07 ms propagates toward the right side and curves due to interference with dust layer. The same trend was observed during experimental investigations of dust lifting behind shock waves by Fan *et al* [9]. The induced flow behind the shock has high temperature, about 670 K. Near the starting point of dust layer, it is seen that the shock-induced flow lifts the dust particles due to a drag force, particle-particle interactions, and the Magnus force. As time passes, the lifting process produces a dust cloud, where gas temperature increases to about 800 K due to the interference between the dispersed dust and the shock-induced flow. Consequently, the coal dust in the dust cloud is heated rapidly and ignites shown at 0.45 ms. After this, flame spreading through the dust cloud induces the ambient coal dust to ignite.

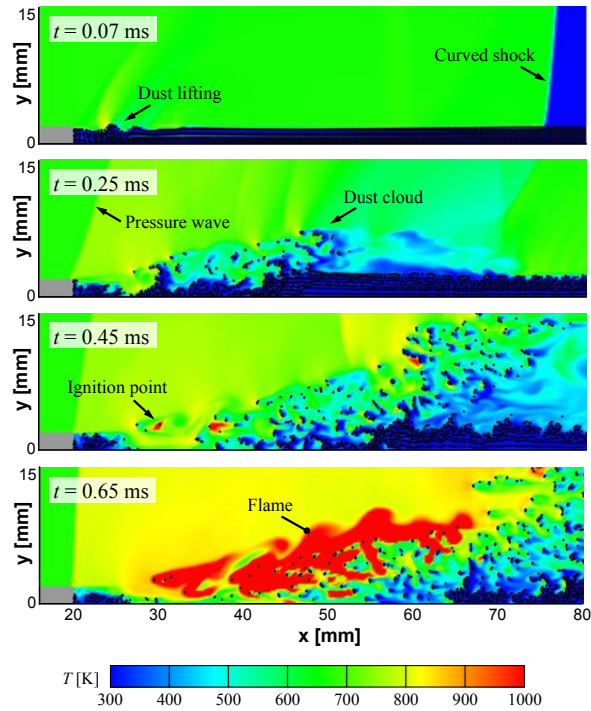


Figure 2. Computed time sequences of gas phase temperature for $O_2 = 24\%$ case in which shock Mach number is 2.60.

In order to discuss the influence of oxygen concentration, flow distributions for the dilute and dense cases are presented in Fig. 3. For the 24% case, high-temperature region in the dust cloud coincides with disappearance of oxygen and appearance of carbon dioxide as shown in Fig. 3 (a). This means that the dispersed dust is heated due to the interference with the shock-induced flow, so that the volatile gas is emitted from the dust particles and starts to combust. In the flame the burnt gas carbon dioxide is produced, and much of the oxygen is consumed from the combustion.

As seen in Fig. 3(b), the same trend can be observed. The dust layer is lifted behind the shock wave and the dust cloud is created. A major difference between the dense and dilute cases is the flame intensity. For the dense case, the flame spread more widely than the dilute one. As presented in Y_{O_2} distributions, the white lines correspond to an equivalence face of methane gas. The oxygen consuming area and the volatile gas emitting area of the dense case are more extensive than that of the dilute case, which may cause the broader flame of the dense case than that of the dilute case. It means that the emitted speed of the volatile gas and the consumption rate of the oxygen increase with increasing oxygen concentration, thus the location of the flame sheet is away from the coal dust. Consequently, the oxygen concentration around dust particles is related to the burning velocity of methane gas. This relation between the flame structure and the oxygen concentration is shown schematically in Fig. 4.

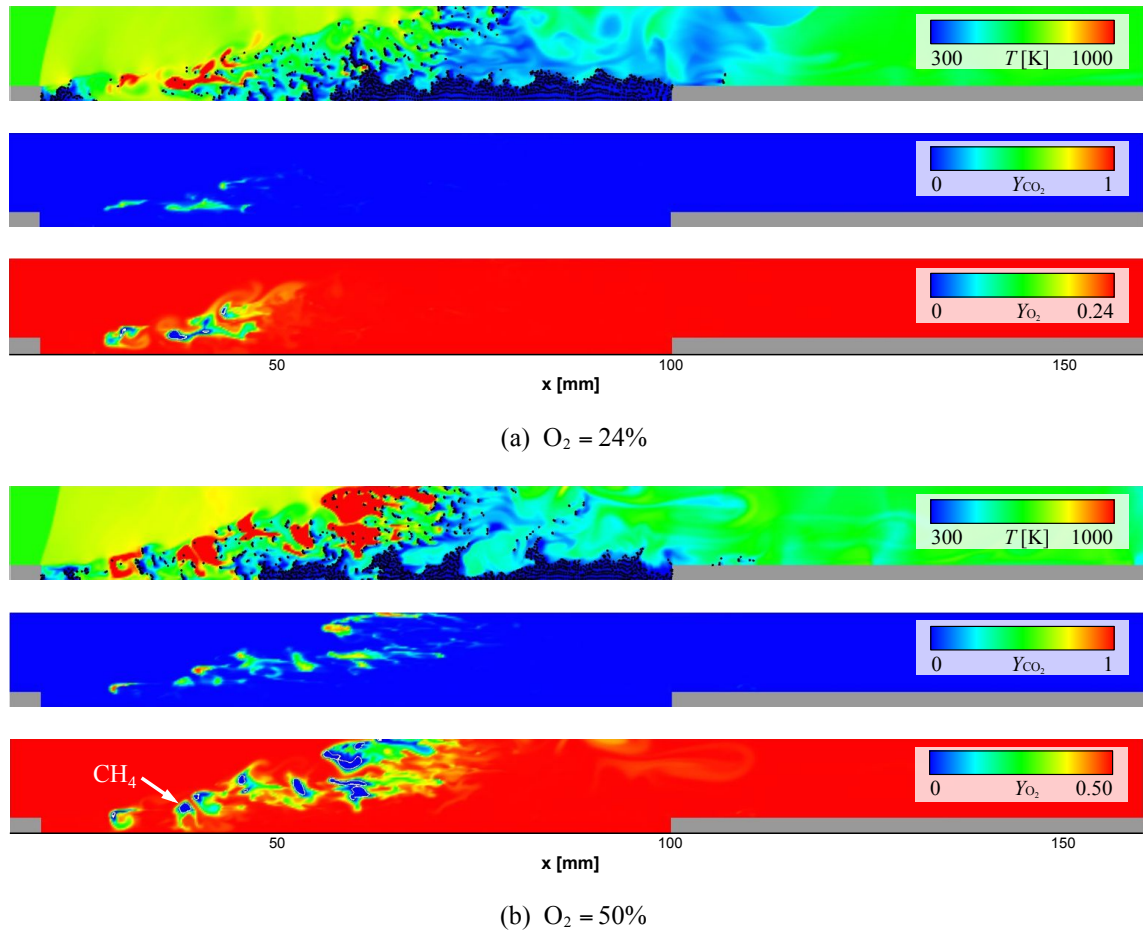


Figure 3. Influence of oxygen concentration on flow distribution for (a) $O_2 = 24\%$ and (b) $O_2 = 50\%$ at a time of 0.50 ms. T , Y_{CO_2} , Y_{O_2} are gas temperature, gas-phase CO_2 mass fraction, gas-phase O_2 mass fraction, respectively. White lines correspond to gas-phase CH_4 mass fraction of 0.01. The height of each frame is 12 mm.

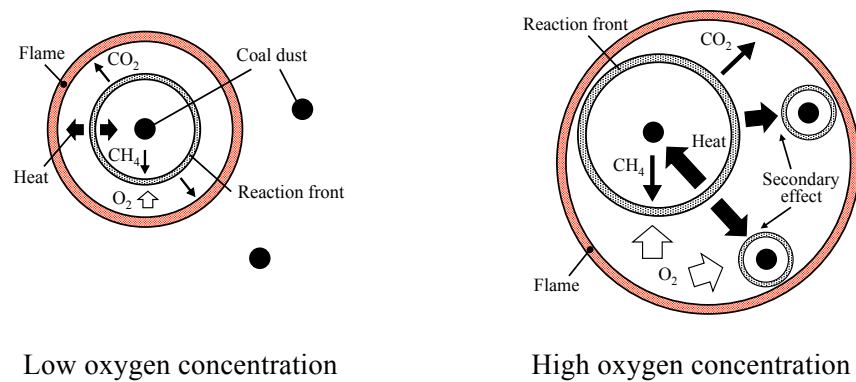


Figure 4. Flame mechanism for layered coal-dust combustion.

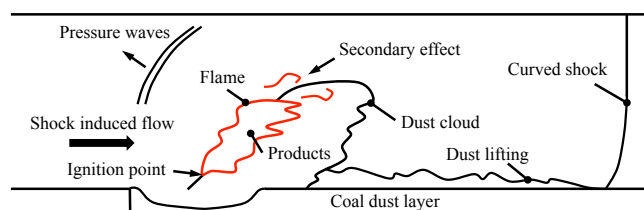


Figure 5. Schematic diagram of a layered coal-dust combustion.

4 Conclusions

In this study, a numerical analysis in the layered coal-dust combustion behind a shock wave was conducted by using numerical simulation based on Euler-Lagrange approach. According to this research the following mechanism as shown in Fig. 5 is important for layered coal-dust explosions behind a propagating shock wave. The shock induced flow lifts the dust layer, producing dust cloud due to drag force, particle-particle interactions, and the Magnus force. The dispersed coal dust is heated rapidly and starts to combust. The location of the flame sheet is subject to the oxygen concentration. In the flame the burnt gas carbon dioxide is produced, and much of the oxygen is consumed from the combustion.

Two cases were considered: a dilute oxygen flow with an initial concentration of 24%, and a dense oxygen flow with an initial concentration of 50%. With increase of oxygen concentration the emitted speed of the volatile gas and the consumption rate of the oxygen increase, so that the location of the flame sheet is away from the coal dust.

Further analysis of layered coal dust explosions for a longer time scale is required to ensure safety of dust explosion hazards, and the additional effect such as Saffman force, non-uniform particle size distribution are taken into consideration in our future work.

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