Detailed numerical simulations of flame propagation in coal-dust clouds

Li Qiao \(^a\) & Jian Xu \(^a\)

\(^a\) School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN, 47907, USA

Available online: 07 Feb 2012

To cite this article: Li Qiao & Jian Xu (2012): Detailed numerical simulations of flame propagation in coal-dust clouds, Combustion Theory and Modelling, DOI:10.1080/13647830.2012.655312

To link to this article: http://dx.doi.org/10.1080/13647830.2012.655312

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.tandfonline.com/page/terms-and-conditions

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.
Detailed numerical simulations of flame propagation in coal-dust clouds
Li Qiao* and Jian Xu

School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907, USA
(Received 11 August 2011; final version received 2 January 2012)

A detailed numerical study was conducted to understand the transient flame propagation process in coal-dust clouds. The model includes detailed chemistry for the gas-phase combustion; devolatilisation kinetics; full coupling between the gas and solid phases; and radiative heat transfer. Furthermore, it solves the gas- and particle-phase momentum equations for the two-phase dynamics. The results show that the flame-speed oscillation phenomenon, which in a previous study was observed for carbon-dust clouds, was not observed for high-volatile coal dust. This is because for high-volatile dusts, such as coal, surface reactions have little impact on flame propagation, which is in fact dominated by volatile combustion. The flame speed largely depends on the devolatilisation rate. For the same reason, neither radiative emission nor absorption is important in high-volatile dust flames because of the much shorter timescale of volatile combustion. The flame structure can be divided into five zones: unburned, preheat, devolatilisation, reaction (gas phase), and post-reaction. Lastly, flame speeds increase when particle size decreases, mainly because the heat released from volatile combustion can be more effectively transported to smaller particles through conduction and convection. This will raise their temperatures more quickly and more profoundly and result in a faster devolatilisation rate and thus faster flame speed.

Keywords: flame propagation speed; dust cloud; detailed chemistry; devolatilisation; radiation absorption and emission

Nomenclature

\( A_p \) particle surface area (cm\(^2\))
\( B_k \) prefactor in the reaction rate expression of surface reaction \( k \)
\( C_{p,i} \) specific heat capacity of species \( i \) (erg g\(^{-1}\) K\(^{-1}\))
\( C_{p,g} \) specific heat capacity of the gas mixture (erg g\(^{-1}\) K\(^{-1}\))
\( C_{p,p} \) specific heat capacity of the particles (erg g\(^{-1}\) K\(^{-1}\))
\( D \) diffusivity (cm\(^2\) s\(^{-1}\))
\( d_p \) particle diameter (cm)
\( E \) activation energy (erg mol\(^{-1}\))
\( F_s \) Stokes forces (dyne)
\( h \) convective heat transfer coefficient (erg cm\(^{-2}\) K\(^{-1}\) s\(^{-1}\))
\( h_i \) specific enthalpy of species \( i \) (erg g\(^{-1}\))
radiation intensity (erg cm\(^{-2}\) s\(^{-1}\))
black-body radiation intensity (erg cm\(^{-2}\) s\(^{-1}\))
radiation intensity along a specific solid angle (erg cm\(^{-2}\) s\(^{-1}\))
thermal conductivity of the gas mixture (erg cm\(^{-1}\) k\(^{-1}\) s\(^{-1}\))
mass (g)
carbon consumption rate as a result of surface reactions (g s\(^{-1}\))
volatile release rate (g s\(^{-1}\))
particle-number density (cm\(^{-3}\))
Nusselt number
pressure (dyne cm\(^{-2}\))
convective heat transfer between a single particle and the bulk gas (erg s\(^{-1}\))
total heat release rate by all gas-phase reactions (erg cm\(^{-3}\) s\(^{-1}\))
gas-phase radiation heat loss (erg cm\(^{-3}\) s\(^{-1}\))
radiative energy absorbed by one particle from the hot gases (erg s\(^{-1}\))
total heat-release rate by all surface reactions (erg s\(^{-1}\))
particle radiation heat loss (erg s\(^{-1}\))
heat of devolatilisation
Re\(_p\) Reynolds number defined using the relative velocity between a particle and the bulk gas
universal gas constant (erg mol\(^{-1}\) K\(^{-1}\))
radius (cm)
particle radius (cm)
enthalpy transfer from particle phase to gas phase because of devolatilisation and surface reactions (erg cm\(^{-3}\) s\(^{-1}\))
temperature (K)
time (s)
gas velocity (cm/s)
particle velocity (cm/s)
diffusion velocity of species \(i\) (cm/s)
molecular weight of carbon (g mol\(^{-1}\))
molecular weight of species \(i\) (g mol\(^{-1}\))
average molecular weight of all gaseous species (g mol\(^{-1}\))
production rate of species \(i\) because of devolatilisation and surface heterogeneous reactions (mol cm\(^{-3}\) s\(^{-1}\))
mole fraction of species \(i\) in the gas mixture
mole fraction of species \(i\) on the particle surface
mass fraction of species \(i\) in the gas mixture
mass fraction of species \(i\) on the particle surface

Greek Letters
emissivity of particle surface
Planck mean absorption coefficient (cm\(^{-1}\))
solid angle
density of the gas mixture (g cm\(^{-3}\))
density of the particle (g cm\(^{-3}\))
viscosity of gas phase (g cm\(^{-1}\) s\(^{-1}\))
species \(i\) production rate resulting from gas-phase reactions (mol cm\(^{-3}\) s\(^{-1}\))
1. Introduction

Flame propagation in gaseous mixtures as a deflagration or detonation wave has been studied extensively in the past few decades. Studies on the combustion of heterogeneous systems such as gas/particle mixtures, however, are relatively sparse. These systems have important practical applications. Many varieties of dust are combustible if dispersed in air with a nearby ignition source, e.g., dusts originating from coal, aluminium, sugar, corn starch, and synthetic materials. But the fundamental mechanisms of flame propagation through combustible dusts are not yet completely understood. The reason for this is mainly due to the complex chemical and physical processes involved, e.g., heterogeneous surface reactions, devolatilisation, combustion of volatiles, molecular transport of species, and heat transfer. The couplings between these different physical and chemical processes make understanding them even more complicated.

Several reviews [1–4] have revealed some important findings of dust flames, though the flame propagation mechanism remains ambiguous. Most numerical studies in literature used simple models with many assumptions; fewer detailed numerical investigations have been reported. Krazinski et al. [5] summarised previous work on the development of dust flame propagation models. Essenhigh and Csaba [6] were among the first to develop a 1-D steady-state flame propagation model based on a thermal theory with a set of assumptions, e.g., the particles and gas have the same velocity, and the detailed devolatilisation and combustion process were neglected. This model was later improved by Bahduri and Bandyopa [7] when they included a heat generation term from chemical reactions. Ozerova and Stepanov [8] developed a 1-D model that considers radiative heat transfer using a so-called differential approximation. Smoot et al. [9] developed a model that considered devolatilisation and subsequent volatile combustion reactions in the gas phase by using relatively simple kinetics, but radiation was neglected in the model. Most recently, Bradley et al. [10] developed a more detailed model for a 1-D laminar, steady-state coal flame by including soot formation and speciated devolatilisation, and the gas-phase reactions used detailed chemistry. This model showed the improved accuracy of its predictions.

Nevertheless, the models used for conservation equations are comparatively simple in the studies mentioned above. For instance, the kinetics for gas-phase reactions are rather simple (except [10]), and many used one-step global kinetics. In some studies, equilibrium gas-phase chemistry was assumed to simulate the burning process. Moreover, many researchers assumed that the gas and particles have the same velocity, which may not be an appropriate approximation because of the large difference in the inertias of gases and particles. Furthermore, radiative heat transfer within the two-phase system was either neglected or modelled in a simple way (e.g., not considering radiative absorption by particles). Lastly, nearly all of these numerical investigations deal with steady-state flame propagation, though the transient process could be more representative of dust ignition and explosion.
Motivated by this, we have developed a detailed model to simulate the transient flame propagation process in a dust cloud. In this model, the gas-phase uses detailed chemistry, variable thermodynamic properties, and multi-component transport properties. It solves gas- and particle-phase momentum equations to obtain the two-phase velocities. Furthermore, radiation absorption and emission by gases and particles are both considered. Lastly, the interactions between the two phases, including species, mass, and energy exchanges, were carefully modelled. The model uses the Eulerian approach; that is, the gases and particles are treated as two interacting continua. Using this model in a previous paper, we discussed the general characteristics of flame propagation in a carbon dust cloud [11]. In particular, we reported and discussed the flame-speed oscillation phenomenon, which had been observed in several two-phase combustion experiments, but the mechanism was not clear. We proposed and demonstrated that the oscillation was caused by a velocity slip between the two phases, which led to a periodic change of the local particle-number density ahead of the flame front, causing flame-speed oscillation.

The present paper is an extension of this previous study – it considers flame propagation in high-volatile dusts such as coal. We have shown that for nonvolatile dusts such as carbon, the mechanisms of flame propagation are dominated by surface heterogeneous reactions that are slower than the gas-phase combustion. Because of the relatively large timescale, radiative emission and absorption are both important in energy transport. In particular, the radiative absorption by unburned particles from the hot reaction and post-reaction zones preheats the unburned mixtures and thus increases the flame propagation speed. These conclusions, however, may be different for high-volatile dusts because combustion of volatiles can be a controlling mechanism in such systems. Thus the flame propagation process depends on the type of volatiles, how fast they are released, and the gas-phase kinetics of volatile combustion. Because the combustion of volatiles in the gas phase is typically much faster than surface heterogeneous reactions, it is possible that radiation heat transfer may not be that important in such flames. Moreover, the devolatilisation process and the subsequent burning of volatiles generally interfere with surface heterogeneous reactions, making the chemical processes in the reaction zone highly complicated. The chemical processes could involve a release of volatiles from particle surfaces, preferential diffusion in the boundary layer, homogeneous combustion of volatiles after premixing with O₂ in the gas phase, diffusional combustion of volatiles without premixing, surface heterogeneous reactions, and other combinations [4]. A detailed numerical simulation that considers these various processes may be able to reveal the fundamental mechanisms of flame propagation, as well as the interactions between the various processes in the reaction zone.

The objective of this paper is to understand the transient flame propagation process in a coal-dust cloud by using detailed numerical simulations. We especially want to determine the detailed flame structure and how various processes interfere/interact with one another in the reaction zone. We also want to quantitatively examine the effects of radiation emission and absorption on flame propagation. Lastly, the effect of particle size on flame propagation speed and flame structure is determined.

2. Model Description
Coal particles with a diameter \(d_p\) and a number density \(N_p\) (number of particles per cm\(^3\)) are uniformly distributed within a cloud. The cloud also contains oxygen and nitrogen. A hot spot is used to ignite the two-phase mixture at the centre. The mechanisms, including mass and heat transport, devolatilisation, and chemical reactions of both phases, establish a flame that propagates outwardly. The transient flame propagation process is modelled
by the conservation equations of mass, species, momentum, and energy of both phases. In these equations, the subscripts \( g \) and \( p \) denote the gas and particle phases, respectively. The time-dependent conservation equations are presented in a spherical coordinate. Several assumptions are applied. Coal particles are assumed to be spherical. The temperature is assumed to be uniform within each particle because of its small size and the large thermal conductivity of particles. The particle diameter decreases with time because of heterogeneous surface reactions. The char porous structure and its evolution were neglected. Under these assumptions, the mass, species, momentum, and energy conservation equations are reduced to 1-D equations in the radial direction.

2.1. Gas-phase conservation equations

In the gas phase, the 1-D governing equations for the conservation of mass, species, and energy in a spherical coordinate are as follows:

\[
\frac{\partial \rho_g}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_g u_g) = N_p m_p \tag{1.1}
\]

\[
\frac{\partial (\rho_g Y_i)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_g u_g Y_i) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_g Y_i V_i) + \dot{\omega}_i + \dot{w}_i \tag{1.2}
\]

\[
\rho_g C_{p,g} \left( \frac{\partial T_g}{\partial t} + u_g \frac{\partial T_g}{\partial r} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 k \frac{\partial T_g}{\partial r} \right) - \sum_{i=1}^{K} \rho_g C_{p,i} Y_i V_i \frac{\partial T_g}{\partial r} - \sum_{i=1}^{K} (\dot{\omega}_i + \dot{w}_i) h_i + Q_{g,rad} + N_p Q_{con} + S_h \tag{1.3}
\]

where \( \rho_g \) is the density of the gas mixture; \( u_g \) is the gas-phase velocity in the radial direction; \( N_p \) is the particle-number density; \( m_p \) is the total mass transfer rate from a single particle as a result of both devolatilisation and surface reactions; \( Y_i \) is the mass fraction of species \( i \); \( W_i \) is the molecular weight of species \( i \); \( \dot{\omega}_i \) is the mass production rate of species \( i \) resulting from gas-phase reactions; \( \dot{w}_i \) is the mass production rate of species \( i \) as a result of both devolatilisation and surface heterogeneous reactions; \( V_i \) is the diffusion velocity of species \( i \); \( C_{p,g} \), is the average specific heat of the gas mixture under constant pressure; \( T_g \) is the gas-phase temperature; \( k \) is the thermal conductivity of the gas mixture; \( h_i \) is the enthalpy of species \( i \); \( Q_{g,rad} \) is the gas-phase radiative heat transfer, including radiative energy emitting and absorbing; \( Q_{con} \) is the convective heat transfer between a particle and the bulk gas; and \( S_h \) is the total enthalpy transfer from the particles to the gases as a result of mass transfer because of devolatilisation and surface reactions.

The left-hand side of Equations (1.1–1.3) includes the time-dependent and convection terms. The right-hand side of Equation (1.1) is the total mass production rate from the particles to the gas phase as a result of devolatilisation and surface heterogeneous reactions. In Equation (1.2), the source terms on the right-hand side represent the production rate of species \( i \) because of molecular diffusion, gas-phase reactions, and mass transfer from the particles which includes both devolatilisation and surface reactions. The source terms on the right-hand side of Equation (1.3) represent thermal conduction, molecular diffusion, enthalpy variation because of species mass generation, radiative energy transfer, and enthalpy transfer as a result of mass transfer between the two phases.
In the gas phase, the equation of state for an ideal gas is

\[ P = \rho_g RT_g / \bar{W} \]  

(1.4)

Using the equation of state and assuming the low mach flow condition, the gas-phase continuity equation, Equation (1.1), can be expressed as [11]

\[- \rho_g \left[ \frac{1}{T_g} \frac{\partial T_g}{\partial t} + \bar{W} \sum_i \frac{1}{W_i} \frac{\partial Y_i}{\partial t} \right] + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_g u_g) = N_p \dot{m}_p \]

(1.5)

The convective heat transfer between a particle and the bulk gas, \( Q_{\text{con}} \), is defined as [12]

\[ Q_{\text{con}} = -h A_p (T_g - T_p) \]

(1.6)

\[ h = \frac{Nuk}{d_p} B \exp(B) - 1, \quad B = \frac{\dot{m}_p C_{p,g}}{\pi d_p Nuk} \]

(1.7)

The Nusselt number was set to have a value of 2 for the present low Reynolds number flow.

The enthalpy transfer between the two phases resulting from surface heterogeneous reactions and devolatilisation is expressed as

\[ S_h = \sum_i \dot{w}_i h_i \]

(1.8)

where \( h_i \) is the specific enthalpy of species \( i \) which participates in the surface reactions or/devolatilisation process.

To account for radiative heat transfer in the two-phase system, the radiative transfer equation (RTE) in the 1-D spherical coordinate was solved [13]:

\[ \frac{\mu}{r^2} \frac{\partial}{\partial r} (r^2 I) + \frac{1}{r} \frac{\partial}{\partial \mu} [(1 - \mu^2)I] = \kappa (I_b - I) \]

(1.9)

where \( I \) is the radiation intensity; \( \mu \) is cosine of the polar angle; \( k \) is the Planck mean absorption coefficient of the gas mixture; and \( I_b \) is the black-body radiation intensity.

The gas-phase radiative heat transfer term can be expressed as

\[ Q_{g,\text{rad}} = -\kappa \left( 4\pi I_b - \int_{4\pi} I d\Omega \right) \]

(1.10)

where \( \int_{4\pi} I d\Omega \) is the incident radiation intensity, and \( \Omega \) is the solid angle. In the present study, the discrete ordinate method (DOM) was used to solve the radiative transfer equation. Once the radiative transfer equations corresponding to various ordinates, see Equation (1.9), are solved, Equation (1.10) is given as

\[ Q_{g,\text{rad}} = -\kappa \left( 4\sigma T_g^4 - \sum_i \omega_i I_i \right) \]

(1.11)
where \( \sigma \) is the Stephan-Boltzmann constant, and \( \omega_i \) is weight of integration corresponding to the \( i \) ordinate, and it satisfies

\[
\int_{4\pi} I d\Omega = \sum_i \omega_i I_i
\]

A different set of \( \omega_i \) should be used according to the total number of ordinates. The Planck mean absorption coefficient of the gas mixture, \( \kappa \), is expressed as

\[
\kappa = \sum_i \kappa_i P_i
\]

where \( \kappa_i \) and \( P_i \) are the Planck mean absorption coefficient and partial pressure of species \( i \), respectively. In the present study, \( \text{CH}_4, \text{CO}_2, \text{CO}, \text{and H}_2\text{O} \) are considered as absorbing and emitting gases, and their Planck mean absorption coefficients were taken from Ref. [12]. It is noted that using Planck mean absorption coefficients usually underestimates the degree of absorption, especially for very slow, near limit flames or when there are strong absorber gases in the mixtures. This has been demonstrated in several previous studies concerning gaseous flames [14–16]. For the present high-volatile dust flames, however, the main radiative heat transport is through particles. As has been shown by many previous studies including the present paper, gas-phase radiation in dust flames is much less important than particle radiation. Due to this consideration, we used Planck mean absorption coefficients instead of the spectral-dependent absorption coefficients which are rather complicated.

### 2.2. Particle-phase governing equations

The particle number density \( N_p \), velocity \( u_p \), density \( \rho_p \), diameter \( r_p \), and temperature \( T_p \) are the five variables to solve. The particle phase is considered as a continuous phase characterised by these variables, and the governing equations are described from Euler’s perspective. The total \( N_p \) is conserved; the conservation equation of \( N_p \) has a similar form as the gas-phase continuity equation. The particle velocity is determined by solving the momentum equation, in which the Stokes force is considered. Gravity force is not considered in the present model.

When coal particles are heated in an oxidiser environment, they experience devolatilisation and surface reactions, which may take place simultaneously. Devolatilisation occurs volumetrically, and heterogeneous reactions take place on particle surfaces. The former process changes particle density and the latter alters particle size [10]. Here, we neglected the porous structure of the char and its evolution during the chemical transformation. We assumed the particle shrank as a result of surface reactions.

The governing equations in the 1-D spherical coordinate are as follows:

\[
\frac{\partial n_p}{\partial t} + \frac{\partial (r^2 N_p u_p)}{\partial r} = 0
\]

\[
m_p \left( \frac{\partial u_p}{\partial t} + u_p \frac{\partial u_p}{\partial r} \right) = F_S
\]

\[
\frac{\partial \rho_p}{\partial t} + u_p \frac{\partial \rho_p}{\partial r} = -\frac{6m_v}{\pi d_p^2}
\]
\[
\frac{\partial d_p}{\partial t} + u_p \frac{\partial d_p}{\partial r} = - \frac{2 \dot{m}_C}{\pi \rho_p d_p^2}
\]

\[
m_p C_{p,p} \left( \frac{\partial T_p}{\partial t} + u_p \frac{\partial T_p}{\partial r} \right) = Q_c + Q_v - Q_{\text{con}} - Q_{p,\text{rad}} + Q_{g,\text{rad}-p}
\]

where \(u_p\) is the particle velocity; \(\rho_p\) is the density of the particles; \(F_S\) is the Stokes force; \(\dot{m}_V\) and \(\dot{m}_C\) are the mass reduction rate of each particle as a result of devolatilisation and heterogeneous reactions, respectively; \(C_{p,p}\) is the heat capacity of particles; \(\dot{Q}_c\) is the overall heat release from all surface reactions; \(Q_v\) is heat needed for the devolatilisation process; \(Q_{\text{con}}\) is the convective heat transfer between a particle and the bulk gases, given by Equation (1.6); \(Q_{p,\text{rad}}\) is the radiative heat loss emitted from the particle surface; and \(Q_{g,\text{rad}-p}\) is the radiative energy absorbed by each particle from the hot gases. The source terms on the right-hand side of Equation (2.5) represent heat release (or absorption) from all surface reactions, heat for devolatilisation, convective heat transfer between a particle and the bulk gases, radiative emission, and radiative absorption by each particle.

For low Reynolds number flows, the Stokes drag force can be expressed as [17]

\[
F_S = 3\pi \mu_g d_p (u_g - u_p) \left(1 + 0.15 Re_p^{0.687} \right)
\]

where \(Re_p\) is the Reynolds number defined using the relative velocity between a particle and the bulk gas, as [17]

\[
Re_p = \frac{\rho_g d_p |(u_p - u_g)|}{\mu_g}
\]

The radiation emission rate from a single particle, \(Q_{p,\text{rad}}\), and the radiative energy absorption rate, \(Q_{g,\text{rad}-p}\), can be expressed as [11]:

\[
Q_{p,\text{rad}} = A_p \varepsilon_p \sigma T_p^4
\]

\[
Q_{g,\text{rad}-p} = \frac{1}{4} A_p \varepsilon_p \int_{4\pi} I d\Omega
\]

where \(\varepsilon_p\) is the emissivity of the particle surface (a value of 1 was used in the present study) and \(A_p\) is the particle surface area.

### 2.3. Coal-particle devolatilisation

The devolatilisation process of coal is a complicated one. The volatile yield and composition are influenced by a number of factors, such as coal type, particle size, heating rate, time-temperature history and pressure [18]. The volatile usually consists of a mixture of combustible gases (\(H_2\), \(CO\), \(CH_4\), \(C_2H_6\), and other hydrocarbons), \(CO_2\), water vapour, soot, tar, \(HCN\), \(NH_3\), \(H_2S\), and possibly a small amount of phenolic and other compounds [10]. Many experiments have been carried out to identify the kinetics of coal devolatilisation. However, the models and rate parameters are diverse because the devolatilisation rate is influenced by a number of factors, including temperature, residence time, pressure, particle size, and coal type [19]. Due to these considerations, we assumed the volatile yield was composed of \(CH_4\) and \(H_2O\) only. The former is a major component of the yielded
Table 1. Reaction rate constants for devolatilisation and char surface reactions.

<table>
<thead>
<tr>
<th>Chemical Reaction</th>
<th>$K = B \exp(-E/RT)$</th>
<th>B (10$^3$)</th>
<th>E (J/mole)</th>
<th>Heat of Reaction (J/Kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Devolatilisation of water [10]</td>
<td>1.00 $\times$ 10$^{13}$ (s)</td>
<td>1.464 $\times$ 10$^5$</td>
<td>-2.257 $\times$ 10$^6$</td>
<td></td>
</tr>
<tr>
<td>Devolatilisation of CH$_4$ [29]</td>
<td>1.14 $\times$ 10$^5$ (s)</td>
<td>7.400 $\times$ 10$^4$</td>
<td>-1.675 $\times$ 10$^6$</td>
<td></td>
</tr>
<tr>
<td>Surface reaction A [20]</td>
<td>1.225 $\times$ 10$^3$ (m/s)</td>
<td>9.977 $\times$ 10$^4$</td>
<td>1.287 $\times$ 10$^6$</td>
<td></td>
</tr>
<tr>
<td>Surface reaction B [20]</td>
<td>1.813 $\times$ 10$^3$ (m/s)</td>
<td>1.089 $\times$ 10$^5$</td>
<td>7.656 $\times$ 10$^6$</td>
<td></td>
</tr>
<tr>
<td>Surface reaction C [20]</td>
<td>7.351 $\times$ 10$^3$ (m/s)</td>
<td>1.380 $\times$ 10$^5$</td>
<td>-3.682 $\times$ 10$^6$</td>
<td></td>
</tr>
</tbody>
</table>

Combustible gases; this assumption has been also used by other papers [20]. Here we want to understand the effects of devolatilisation and the combustion of volatiles on flame propagation speed and flame structure. However, we tested the sensitivity of the amount of CH$_4$ in the volatile on flame speed and structure. This will be discussed in section 3.5.

The devolatilisation rate is modelled as a one-step global reaction, and the mass reduction rate is expressed as [10]

$$\dot{m}_i = -k_i m_i$$  \hspace{1cm} (3.1)

where $i$ denotes the volatile species (H$_2$O and CH$_4$); $m$ is the remaining mass of the volatiles in the particle; $k$ is the rate constant, which is correlated with the particle temperature $T_p$ as

$$k_i = B_i \exp\left(-\frac{E_i}{RT_p}\right)$$  \hspace{1cm} (3.2)

where $B$ is the frequency factor, $E$ is the activation energy, and $R$ is the universal gas constant.

The total volatile mass reduction rate used in Equation (2.3) can be expressed as

$$\dot{m}_V = -(\dot{m}_{H_2O} + \dot{m}_{CH_4})$$  \hspace{1cm} (3.3)

The rate constants and the references from which they were obtained are listed in Table 1.

2.4. Particle surface reactions

Several chemical reactions may occur on the surface of a coal particle, depending on the gases surrounding the particle. Here we considered the three most important surface reactions:

\[ C + O_2 \rightarrow CO_2 \]  \hspace{1cm} (A)
\[ 2C + O_2 \rightarrow 2CO \]  \hspace{1cm} (B)
\[ C + CO_2 \rightarrow 2CO \]  \hspace{1cm} (C)

The global rate for each reaction was simulated by using the diffusion-kinetic model [21], which is the first order of the gaseous species in the reactants. The reaction rates for reactions
A, B, and C can be expressed as

\[ R_k = -A_p \rho Y_{k,s} B_k \exp \left( -\frac{E_k}{RT_p} \right) \]  

(4.1)

where subscription \( k \) denotes reactions A, B, and C; \( Y_{k,s} \) is the mass fraction of the gas-phase reactant at the particle surface; \( B_k \) is the pre-factor; and \( E_k \) is the activation energy. The kinetic constant and the references from which they were obtained are listed in Table 1.

According to Equation (4.1), the total consumption rates of carbon, \( \text{O}_2 \), and \( \text{CO}_2 \) can also be expressed as a function of the surface mass fraction \( Y_{\text{O}_2,s} \) and \( Y_{\text{CO}_2,s} \). Based on mass balance, the \( \text{O}_2 \) and \( \text{CO}_2 \) concentrations at a particle surface can be expressed as [20]

\[ Y_{\text{O}_2,s} = -\frac{\dot{m}_{\text{O}_2,s}}{\dot{m}_p} + \left( Y_{\text{O}_2,\infty} + \frac{\dot{m}_{\text{O}_2,\infty}}{\dot{m}_p} \right) \exp (-B_{\text{O}_2}) \]  

(4.2)

\[ Y_{\text{CO}_2,s} = -\frac{\dot{m}_{\text{CO}_2,s}}{\dot{m}_p} + \left( Y_{\text{CO}_2,\infty} + \frac{\dot{m}_{\text{CO}_2,\infty}}{\dot{m}_p} \right) \exp (-B_{\text{CO}_2}) \]  

(4.3)

where \( Y_{\text{O}_2,\infty} \) and \( Y_{\text{CO}_2,\infty} \) are the mass fractions of \( \text{O}_2 \) and \( \text{CO}_2 \) in the gas phase, respectively, \( B_{\text{O}_2} \) and \( B_{\text{CO}_2} \) are the transfer number, which is expressed as

\[ B_i = \frac{\dot{m}_p}{\pi d_p N u_p D_{im}} \]  

(4.4)

where \( i \) denotes species \( \text{O}_2 \) and \( \text{CO}_2 \). \( D_{im} \) is the mass diffusivity of species \( i \) and \( \dot{m}_p \) is the total mass flux (\( \dot{m}_p = \dot{m}_C + \dot{m}_V \)).

Given the mass fraction of \( \text{O}_2 \) and \( \text{CO}_2 \) in the gas phase (\( Y_{\text{O}_2,\infty} \) and \( Y_{\text{CO}_2,\infty} \)), Equations (4.1) to (4.4) form a closed system of unknowns, \( Y_{\text{O}_2,s} \) and \( Y_{\text{CO}_2,s} \). The nonlinear equation system is solved using the DNEQN solver in the IMSL library [22]. The solver uses a modified Powell hybrid algorithm and a finite-difference approximation to the Jacobian matrix. Once \( Y_{\text{O}_2,s} \) and \( Y_{\text{CO}_2,s} \) are obtained, the consumption rates of carbon, \( \text{O}_2 \) and \( \text{CO}_2 \) (\( \dot{m}_C, \dot{m}_{\text{O}_2,s} \) and \( \dot{m}_{\text{CO}_2,s} \)), can also be determined.

### 2.5. Boundary conditions and initial conditions

The two-phase system has a variable set as \( (u_g, T_g, Y_1, \ldots, Y_N, N_p, u_p, T_p, d_p) \), where \( N \) is the total number of gas-phase species. The size of the computational domain is 10 cm with the left boundary at the centre of the sphere (\( R_L = 0 \) and \( R_R = 10 \) cm). The following boundary conditions were used.

Left boundary (centre of the sphere):

\[ u_g = u_p = 0 \text{ and } \frac{d\phi}{dr} = 0, \text{ the variables are } \phi, \text{ except } u_g \text{ and } u_p \]

Right boundary (outer domain boundary):

\[ \frac{d(r^2 \rho u_g)}{dr} = \frac{d(r^2 n_p u_p)}{dr} = 0 \]

\[ \frac{d\phi}{dr} = 0, \text{ the variables are } \phi, \text{ except } u_g \text{ and } u_p \]
Various initial conditions can be assigned to the system. For the present study, initially, both gas and particle phases are stationary, and a uniform gas and particle field was used, which gives:

\[ \mathbf{u}_g = \mathbf{u}_p = 0, \phi = \phi_0 \text{ (other solution variables are } \phi) \]

The ignition of dust flow requires a much larger ignition kernel volume and a much longer ignition time than the ignition of a gaseous mixture [4]. In the present modelling, a hot spot was used to ignite the dust mixture. The hot spot is at the centre of the sphere and has a diameter of 0.8 cm. The volumetric heating rate of the hot spot is 20 W/cm\(^3\), and the duration of the heating is 0.06 second. The total ignition energy supplied by the hot spot is about 0.64 joule.

2.6. Gas-phase reactions, physical properties and numerical method

The detailed mechanism of GRI-Mech 1.2 [23] was applied for the gas-phase reactions used. The transport and thermodynamics properties of all gaseous species were taken from the CHEMKIN database. The CHEMKIN subroutines [24] were used to calculate the gaseous chemical reaction rates, specific heats, enthalpies, diffusive velocities, viscosities, and thermal conductivities.

The time-dependent governing equations for both phases were solved simultaneously by using a finite differencing method. A second-order central differencing was used for all diffusive terms, and a third-order upwind QUICK scheme was used for the convective terms in all equations. The discretised gas-phase and particle-phase equation system was then integrated by the use of DASPK [25], which is capable of solving stiff differential-algebraic equations (DAE). The time-step size was automatically adjusted by a DASPK solver based on the characteristics of the system. In the present study, the smallest time-step size is about \(10^{-7}\) second, and up to the fifth-order time discretisation was used.

In the reaction zone, solution variables such as temperature, particle-number density, and particle size have large gradients; thus a small grid size is required. To resolve the detailed flame structure there and to reduce the total number of grid points in the computational domain, we also implemented an adaptive mesh strategy. Computational grid points can be added or removed, based on gas-phase and particle-phase temperatures, velocity, and particle-phase number density.

3. Results and discussion

3.1. Time histories

Numerical simulations were performed for various coal/air mixtures to investigate the transient flame propagation process, the detailed flame structure, and the influence of two-phase dynamics, radiative heat transfer, and particle size on the burning process. All simulations were performed for small coal particles (in the range of 10–100 \(\mu m\)) at moderate concentrations. Very low or high concentrations were not considered because such flames may be difficult to ignite; in reality, they would need assistance of a combustible gas such as \(CH_4\) to be present in the initial mixture.

The discussions that follow are for a dust cloud containing coal particles with a number density of 12,000 cm\(^{-3}\) and a diameter of 30 \(\mu m\). The cloud also contains 30% \(O_2\) and 70%
Table 2. Approximate analysis of the coal.

| Moisture (%) | 16.15 |
| Volatile matter (%) | 42.59 |
| Carbon (%) | 40.23 |
| Ash (%) | 1.03 |
| Density (g/cm³) | 1.3 |

N₂ at atmospheric pressure and room temperature. The coal chosen is Illinois No. 6 coal, and its properties are listed in Table 2. The calculated fuel equivalence ratio is about 1.5.

3.1.1. Temperature

Figure 1 shows profiles of the gas and particle temperatures $T_p$ and $T_g$ as a function of radius at four selected times. $T_g$ is higher than $T_p$ in the reaction zone and the post-reaction zone. The difference is most significant in the reaction zone. For instance, at $t = 0.131$ s the peak $T_g$ is about 2280 K, but the peak $T_p$ is about 1920 K. Further, the peak $T_p$ and $T_g$ do not coincide: the peak of $T_g$ appears earlier than that of $T_p$ with respect to the unburned mixture. The gases in the reaction zone experience a sharp increase in temperature as a result of gaseous combustion. This temperature rise is faster for the gases than for the particles. Note the temperatures near the centre of the sphere are high at early stage, which is a result of the ignition energy posed at the centre to assist the ignition.

The unburned $T_p$ and $T_g$ remain the same as the ambient temperature, 300 K. Preheating of unburned particles was not observed here. This is different from the carbon dust clouds we studied previously [11]. For the carbon dust clouds, $T_p$ and $T_g$ of the unburned mixture

Figure 1. Profiles of the gas and particle temperatures as a function of radius at selected times. The particle number density is 12,000 cm$^{-3}$, and the particle diameter is 30 µm. The dust contains 30% O₂ and 70% N₂ initially.
can be elevated by a few hundred Kelvin degrees because the unburned particles absorb radiative energy from the hot flame. The preheating consequently results in faster flame propagation speed. For the present case, however, radiative preheating seems unimportant. We will discuss the effects of radiation absorption and emission in detail in Section 3.3. Another observation is that the peak $T_p$ and the peak $T_g$ both increase with time. This will be explained shortly.

3.1.2. Flame propagation speed

The propagation speed is an important parameter of dust flames. It is defined as $dR/dt$, and $R$ denotes locations where the gas-phase temperature is at a monitor temperature. For the current study, the monitor temperature was set at 1000 K. We have found that the propagation speed is independent of the monitor temperature, except in the ignition region where the flame is highly unstable [11]. Figure 2 shows the flame propagation speed $U$ as a function of radius. During ignition, both the gases and the particles in the ignition zone are heated. The combustible volatile (CH$_4$) is released and rapidly mixed with O$_2$. When the temperature of the gas mixture reaches a critical value, homogeneous auto-ignition occurs. This process can be considered as a gaseous explosion, which leads to a high gas-phase velocity. The gas-phase velocity depends on the size of the ignition zone and the heating rate. After this quick gas expansion, the flame velocity drops. In the later stage, the flame speeds reaches a quasi steady state and increases only slightly with time.

It is noted that the flame-speed oscillation phenomenon, which is the alternate mode of fast and slow propagation of the flame front, was not observed for the present study. This phenomenon has been observed by several two-phase combustion experiments. For example, Hanai et al. [26] reported this phenomenon for flame propagation in

![Figure 2](image-url)  
**Figure 2.** The flame propagation speed as a function of radius. The particle number density is 12,000 cm$^{-3}$, and the particle diameter is 30 µm. The dust contains 30% O$_2$ and 70% N$_2$ initially.
polymethylmethacrylate/air dust clouds using a microgravity facility. In our previous numerical study [11], we also found this phenomenon for carbon-dust clouds. Using a detailed numerical analysis, we had demonstrated that the oscillation was caused by a velocity slip between the two phases, which resulted in a periodic change of particle number density at the flame front. This consequently changed the local fuel-equivalence ratio, resulting in flame-speed oscillation. For the present simulations, which deal with high-volatile dusts, however, the oscillation behaviour was not observed, though a velocity slip between the two phases did take place. This will be elaborated on in the following.

3.1.3. Gas and particle velocities and particle-number density

Many numerical studies of dust flames assume that particles and gases have the same velocity. However, because particles have much larger inertia than gases, their velocities can be very different. The velocity slip between the two phases may have an important impact on the fluid dynamics of the system and consequently will affect the burning process [17]. In the following, we will discuss the two-phase dynamics of the dust flame.

Figure 3 shows the profiles of the gas and particle velocities $U_g$ and $U_p$ as functions of radius at selected times. $U_g$ and $U_p$ are approximately equal in the post-reaction zones. This is because the diameter of the particles in this zone is nearly zero (they have been burned); thus the velocity slip, which is a result of the different inertia between the particles and gases, is negligible. In the unburned region, however, $U_g$ is higher than $U_p$. This means that the gases ahead of the flame front move faster than the particles.

Figure 4 shows the profiles of the particle number density $N_p$ for the same dust mixture. The vertical lines represent the locations of the maximum heat release from gas-phase combustion at each occurrence. They suggest where the reaction zone is at each time.

---

Figure 3. Profiles of the gas and particle velocities as a function of radius at selected times. The particle number density is $12,000 \text{ cm}^{-3}$, and the particle diameter is $30 \mu\text{m}$. The dust contains 30% $\text{O}_2$ and 70% $\text{N}_2$ initially.
The value of $N_p$ decreases from right (unburned zone) to left (post-reaction zone), and it experiences a jump across the reaction zone. This is similar to a premixed gaseous flame, for which the density has a jump across the flame zone as a result of thermal expansion. A spike is observed just ahead of the flame front. This is because $U_p$ in the reaction zone is faster than in the unburned region, which causes an accumulation of particles on the right side of the reaction zone. In the unburned region (far right), the $N_p$ value approaches the initial value of 12,000 cm$^{-3}$. A final observation is that the $N_p$ values in the pre-heat and reaction zones decrease monotonically with time (see the $N_p$ values that intercross with the vertical lines). In the following we will explain why the flame-speed oscillation was not observed for high-volatile dusts such as coal, whereas it was observed for nonvolatile (or low-volatile) dusts such as carbon.

For flame propagation in a carbon-dust cloud, we observed a periodic sign change of the relative velocity between the two phases ahead of the flame front [11]. In other words, the gases are moving faster than the particles at one time, but slower the next time. This causes the local particle number density ahead of the flame front to change periodically. For example, the gases are moving faster than the particles initially due to thermal expansion. This causes the particle number density ahead of the flame front to decrease, which is equivalent to a decrease in the local fuel equivalence ratio. As a result, the rate of surface reactions, and consequently the heat release by both the gas-phase and the particle-phase reactions, will decrease. This decrease in reaction intensity will reduce both the gas and the particle velocities. However, gas responses are much faster than those by particles. As a result, the particles are now moving faster than the gases, and this essentially increases the particle number density ahead of the flame front. The consequence is that the reactions become intensified because of a higher number density. This causes more heat release and increases the gas and particle velocities, but the gas velocity increases more than the
particle velocity does. These alternating changes of gas and particle velocities cause a periodic change of local particle-number density (that is, the local fuel equivalence ratio), and consequently it causes flame-speed oscillation.

For the present simulations dealing with high-volatile dusts, however, the gases ahead of the flame front always move faster than the particles (see Figure 3). Further, the particle velocity ahead of the flame front increases monotonically with time. This results in a monotonic decrease of \( N_p \) in the preheat and reaction zones, as shown in Figure 4. This decrease differs from the carbon dust case, for which the \( N_p \) in the reaction zone showed a periodic increase and then a decrease.

In summary, from the perspective of the relative motion between the two phases, major differences exist between nonvolatile dusts and high-volatile dusts. For the former, flame propagation speed is largely determined by particle surface reactions, whereas the gas-phase is more submissive; it acts as a media to carry energy along by heat conduction. For high-volatile dusts, however, flame propagation is largely controlled by the gas-phase reactions or combustion of volatiles. The heat release from volatile combustion continuously accelerates the gases. This heat release also accelerates the particles through heat convection and radiation, but the particles can never be faster than the gases because of their larger inertia. Also, the heat release from surface reactions is much smaller than the gas-phase volatile combustion. In such systems, the gas-phase is more active, controlling the two-phase dynamics and reaction intensity. As a consequence, flame speed oscillation was not observed, even though a velocity slip between the two phases existed.

3.1.4. Reaction rates

In this section, we will explain why flame propagation speed increases slightly with time, as shown in Figure 2, by looking into the reaction rates of several processes, including devolatilisation, combustion of volatiles, and surface heterogeneous reactions. From the above discussions, we have shown that the peaks \( T_p \) and \( T_g \) both increase with time (Figure 1). The \( N_p \) value in the reaction and preheating zones decreases with time (Figure 4).

Figure 5 plots the volumetric heat release rate from volatile combustion (\( Q_g \)), the heat absorption rate because of devolatilisation (\( Q_v \)), and the heat release rate because of surface reactions (\( Q_c \)). Note that \( Q_g \) has a unit of erg/cm\(^{-3}\)s because it is the gas-phase volumetric heat release rate; \( Q_v \) and \( Q_c \) both have a unit of erg/s because they are for a single particle. It can be seen that \( Q_v \), which has a negative sign, increases with time. This is expected because the particle temperature increases with time. \( Q_c \), which also has a negative sign, does not change much with time. It is much smaller than \( Q_v \), indicating that the char-surface reaction rates are much smaller than the devolatilisation rate. Another difference between \( Q_v \) and \( Q_c \) is that \( Q_v \) has values only in the devolatilisation zone (which includes the gas-phase reaction zone), whereas \( Q_c \) also has values in the post-reaction zone. This indicates that slow chemical reactions are maintained in the post-reaction zone after the flame has passed by.

As shown in Figure 5, the heat release rate from the combustion of volatiles \( Q_g \) decreases with time. However, the peak gas temperature \( T_g \) increases with time (Figure 3). We have shown earlier that as a result of thermal expansion, the particle number density \( N_p \) in the reaction and post-reaction zones decreases with time (Figure 4). This indicates that the total volatile release (CH\(_4\)), which should be proportional to \( N_p \), decreases with time. We then examined CH\(_4\) concentration in the post-reaction zone, and it was found to decrease with time. Note after the volatile is released, it rapidly mixes with forming a premixed flame. Additionally, O\(_2\) has a fixed concentration of 30% in the unburned mixture, and the present...
Figure 5. Profiles of the volumetric heat release rate of volatile combustion, the heat absorption rate because of devolatilisation for each particle, and the heat absorption rate because of surface reactions for each particle. The particle number density is 12,000 cm$^{-3}$, and the particle diameter is 30 µm. The dust contains 30% O$_2$ and 70% N$_2$ initially.

simulation is a fuel-rich case. Thus, the effect of the decreased CH$_4$ concentration is that it makes the premixed flame become more stoichiometric as the flame propagates outwardly. Therefore, the peak gas temperature $T_g$ increases with time and the flame propagation speed slightly increases with time (Figure 2). However, $Q_g$ decreases with time because the total volatile release (CH$_4$) decreases as a result of decreased $N_p$.

3.2. Detailed flame structure

So far we have discussed the transient flame propagation process, including flame propagation speed, time histories of the gas and particle temperatures and velocities, particle-number density, and reaction rates. We will now discuss the detailed flame structure. As mentioned earlier, the present model includes detailed gas-phase chemistry; devolatilisation kinetics; simplified particle surface chemistry; full coupling between the two phases, including mass, species, and energy transfer; and also radiative heat transfer between them. Thus it provides better insight into the detailed structure of a dust flame.

Figure 6 shows the structure of the dust flame we have discussed at a selected time $t = 0.131$ s. The flame front is located at approximately $R = 7.5$ cm. Figure 6 (a) shows the profiles of the gas and particle temperatures ($T_p$ and $T_g$) and the concentrations of major species, including CH$_4$, CO$_2$, CO, H$_2$, O$_2$, and H$_2$O. Figure 6 (b) shows the volumetric heat release rate of volatile combustion $Q_g$ and the concentrations of intermediate species, including H, O, OH, and CH$_3$. Figure 6 (c) shows the production rate of volatile species including CH$_4$ and H$_2$O, and carbon mass consumption rates as a result of three surface reactions, all for one particle. Figure 6 (d) shows the profiles of the gas and particle velocities ($U_g$ and $U_p$) and the particle number density $N_p$. 
Figure 6. Detailed structure of the coal dust flame at $t = 0.131$ s: (a) profiles of the gas and particle temperature and concentrations of major species; (b) profiles of the heat release rate of volatile combustion and concentrations of intermediate species; (c) profiles of the production rate of volatile ($\text{CH}_4$ and $\text{H}_2\text{O}$) and the carbon mass consumption rate because of surface reactions; (d) profiles of the gas and particle velocities and particle number density. The particle number density is $12,000 \ cm^{-3}$, and the particle diameter is $30 \ \mu\text{m}$. The dust contains $30\% \ O_2$ and $70\% \ N_2$ initially.

When the flame propagates outwardly, the particles ahead of the flame front are heated rapidly, and devolatilisation takes place. The released volatile ($\text{CH}_4$) rapidly mixes with the $O_2$ in the preheat zone, forming a premixed $\text{CH}_4/O_2$ flame. This burns in a premixed-flame mode, as indicated by the heat-release rate of volatile combustion $Q_g$. Oxygen may diffuse onto the particle surface, and surface reactions may take place, which establish many individual diffusion flames. Viewing from the left side of the reaction zone, we find that $\text{CH}_4$ concentration decreases all the way to zero; from the right side we find that $O_2$ concentration decreases all the way to zero. The concentrations of CO and $H_2$, which are the result of char-surface reactions and gas phase reactions, show the same trend as $\text{CH}_4$.

Figure 6 (c) shows that the production rates of volatiles (including $\text{CH}_4$ and $\text{H}_2\text{O}$) are much larger than the consumption rate of carbon because of char-surface reactions. This indicates that devolatilisation is much faster and more dominant than the surface reactions, and the former would have a more significant impact on flame propagation. $\text{H}_2\text{O}$ is released from the coal particles earlier than $\text{CH}_4$ because it is easier to gasify. The $T_p$ curve has two flat areas, which are caused by devolatilisation of water and $\text{CH}_4$, which absorb energy and thus reduce the particle temperature. Among the three surface reactions, Reaction C is dominant, and Reactions A and B can be neglected. This means that the overall effect of
all surface reactions is to convert CO$_2$ to CO, and CO is then combusted in the gas phase. This is consistent with the double-film theory proposed by Spalding [27].

The devolatilisation zone is wider than the thin gas-phase reaction zone; the latter sits on the right edge of the former. This is more obvious for larger particles, as will be discussed later. This indicates that the particles continue to release volatiles even after the flame has passed through them because the timescale of volatile combustion is much shorter than that of devolatilisation. Furthermore, the particle-reaction zone is much wider than the devolatilisation zone. It extends to the post-reaction zone, indicating that surface reactions continue to take place downstream of the flame, though the reaction rate is much smaller. The reaction that is responsible for this is CO$_2$ + C = 2CO. According to these profiles, we can divide the flame structure into several zones; this is illustrated in Figure 7.

3.3. Effect of radiation emission and absorption

We have shown earlier that for nonvolatile dusts, flame propagation is slower than gaseous flames because it is controlled by surface reactions, which are relatively slow; thus radiation emission and absorption are both important. In particular, the radiation absorption by unburned particles can preheat the unburned mixture by a few hundred Kelvin degrees. On the other hand, the radiation heat loss from the reaction and post-reaction zones to the cold ambient is also significant. All of these results come about because the timescale of chemical reactions is relatively large for such dusts. For high-volatile dusts, however, the dominant mechanism of flame propagation is the combustion of volatiles, which is a faster process than surface heterogeneous reactions. Thus the effect of radiation on flame propagation can be different. In the following, we discuss quantified radiative heat transfer in the two-phase system.

Figure 8 shows the source terms of the gas-phase energy equation for the same dust flame at $t = 0.131$ s, including heat conduction, diffusion, heat release by gas-phase reactions, radiation heat loss, and convective heat transfer. In terms of energy transfer in the gas phase, chemical reaction and conduction are the most important. Convective heat transfer
between the two phases and the diffusion heat are the second most important. The gas-phase radiation heat loss can be neglected.

Figure 9 shows the source terms in the particle energy equation for the same dust flame at $t = 0.131$ s, including convective heat transfer, radiation emission, radiation absorption, heat release by surface reactions, and enthalpy loss resulting from devolatilisation. For particles, the most important mechanisms of energy transport are convection (from gases to particles) and heat loss because of devolatilisation which decreases the particle temperature. The radiation heat loss from the hot particles to the cold ambient is small. The radiation absorption by unburned particles is negligible.

3.4. **Effect of particle size**

Particle size has an important impact on dust ignition and explosion. Particle size could have an impact on multiple physical processes, and these processes could compete with each other. For example, particle size could impact the way chemical reactions take place. Huang et al. [28] showed that as the aluminium particle size decreases from micron to nanoscale, the surface reactions transit from diffusion-controlled to kinetic-controlled because the effective rate of oxygen diffusion onto the particle surface increases as the particle diameter decreases. Furthermore, particles of various sizes may have different heat transfer behaviours in the forms of conduction, convection, and radiation. For instance, larger particles may absorb more radiation energy than smaller particles do, which could affect the devolatilisation behaviour. On the other hand, heat conduction may become more important as the particle size decreases, which could also affect devolatilisation. In the following, we will identify the controlling mechanisms on the effect of particle size.
Figure 9. Profiles of the source terms of the particle-phase energy equations, including convection heat transfer between a particle and the bulk gases, radiation heat loss, radiation absorption, reaction heat due to surface reactions, and devolatilisation heat.

Figure 10 compares the flame propagation speeds of six dust mixtures with varying particle sizes of 10, 20, 30, 40, 50, and 60 µm, respectively. For the purpose of comparison, we keep the overall fuel-equivalence ratio the same. This means that the particle number density is higher for the mixture with smaller particles. The speed decreases as the particle size increases. For instance, the speed for 10 microns is about five times greater than that for 60 microns. This trend is consistent with the experimental and theoretical results in literature on the effect of particle size. For all six, the speed increases slightly with time.

For high-volatile dusts, flame propagation is largely controlled by volatile combustion. Because volatile combustion is usually faster than devolatilisation, the flame propagation speed is very likely determined by the release rate of volatiles. Motivated by this, we compared the volumetric volatile production rate (moles/cm³) as a function of time for the six mixtures. The results are shown in Figure 11. It is clear that the volatile production rate increases with decreasing particle size, which explains the same trend we observed for flame speed.

To further understand the effect of particle size on dust-flame propagation, we compared the flame structure of two dust mixtures having a particle size of 10 µm and 60 µm, respectively. The results are shown in Figure 12 (the figures on the left are for 10 µm and on the right are for 60 µm). Both structures were taken at the flame front located around R = 7.5 cm.

Figure 12 (a) compares the profiles of temperatures and species concentrations. First of all, the difference between $T_p$ and $T_g$ in the reaction zone is larger for the 60-µm dust than for the 10-µm dust. In other words, the particle temperature in the reaction zone is higher for the dusts with smaller particles. This indicates that the heat release from volatile combustion can be more effectively transported to smaller particles than to larger ones by means of conduction and convection. This increases the particle temperature more
quickly and thus increases the devolatilisation rate. Note that the CH$_4$ mole fraction in the post-reaction zone is approximately zero for the 10-µm dust, and it is about 0.15 for the 60-µm dust. This indicates that for the 10-µm dust, the devolatilisation rate is as fast as the combustion rate, thus no volatile is present in the post-reaction zone.
Figure 12. A comparison of flame structure of two dust flames: left figures are for a 10-µm dust; right figures are for a 60-µm dust. (a) profiles of the gas and particle temperatures and major species concentrations; (b) profiles of the heat release rate from volatile combustion and profiles of the concentrations of intermediate species; (c) profiles of the volumetric production rate of volatile species and profile of the carbon consumption rate resulting from surface reactions; (d) profiles of the particle and gas velocities and the particle-number density.
L. Qiao and J. Xu

Figure 12 (b) compares the profiles of the heat release rate resulting from volatile combustion $Q_g$, as well as the concentrations of the intermediate species. The peak $Q_g$ for the 10-µm dust is about six times higher than that for the 60-µm dust. We also observed that the gas-phase reaction zone is narrower for the 10-µm dust than the 60-µm dust.

Figure 12 (c) compares the profiles of the total volumetric production rate of volatiles, including CH$_4$ and H$_2$O, as well as the total consumption rate of carbon as a result of surface heterogeneous reactions. The results show that the devolatilisation zone of the 10-µm dust is narrower than that of the 60-µm dust, and the volumetric production rate of CH$_4$ is five times higher.

Figure 12 (d) compares the profiles of the gas and particle velocities ($U_p$ and $U_g$) and the particle-number density $N_p$. For the 10-µm dust, $U_g$ and $U_p$ are approximately equal. The difference between $U_g$ and $U_p$ is larger for the 60-µm dust because of the larger inertia. $U_g$ ahead of the flame front is larger than $U_p$, indicating that because of thermal expansion, the gases ahead of the flame front move faster than the particles.

In summary, the above analysis shows that the main reason for the significantly increased flame speed at decreased particle size is because heat can be more effectively transported to smaller particles by conduction and convection. This increases the particle temperature more rapidly and profoundly and thus increases the devolatilisation rate, resulting in a faster flame speed.

3.5. Sensitivity analysis

To further identify the controlling mechanisms of flame propagation in high-volatile dust clouds, we performed sensitivity analyses of flame speed with respect to the rate of several processes, including surface heterogeneous reactions, devolatilisation, and heat transfer. We also examined the sensitivity of flame speed with respect to volatile composition—the total amount of CH$_4$ being released. This would help determine the relative importance of these various processes on flame propagation speed. This was evaluated from a series of calculations that perturbed the rate of these processes in question. The results were then used to compute the logarithmic sensitivities by determining the derivatives

$$A_i = \frac{R_i \partial U}{U \partial R_i}$$

where $A_i$ is the sensitivity coefficient, $U$ is the flame propagation speed, and $R_i$ is the reaction rates of three surface reactions A–C, the devolatilisation rates of H$_2$O and CH$_4$, and the rate of heat conduction (gas-phase), respectively. These rates were artificially perturbed by ±10%, and the resulting flame speeds were used to calculate the sensitivity coefficients. Note the flame speed was obtained by averaging its values when the flame front was between 3 cm and 8 cm. For the sensitivity with respect to volatile composition, the total amount of CH$_4$ was artificially changed by ±10% and the resulting flame speeds were used to calculate the sensitivity coefficient.

The results are shown in Figure 13. It can be seen that the flame speed is most sensitive to the heat conduction rate, and secondly sensitive to the total amount of CH$_4$ and the devolatilisation rate of CH$_4$. The coefficients with respect to the reaction rates of three surface reactions and the devolatilisation rate of H$_2$O are very small. It is noted that the present case is at a slightly fuel rich condition; changing the total amount of CH$_4$ means changing the gas-phase equivalence ratio as CH4 is the only combustible volatile, thus the sensitivity coefficients for very lean or very rich flames may be quite different from the
Figure 13. Logarithm sensitivity coefficients of the flame propagation speed with respect to the rates of surface reactions A, B and C, the devolatilisation rate of CH$_4$ and H$_2$O, and the rate of conduction heat transfer, as well as the amount of CH$_4$ being released from the coal. The particle number density is 12,000 cm$^{-3}$, and the particle diameter is 30 $\mu$m. The dust contains 30% O$_2$ and 70% N$_2$ initially.

value obtained for the present case. Additionally, we have shown previously that radiative heat transfer is not important for the present high-volatile dust flames. Thus, the processes that most control flame propagation speed through dust clouds are heat conduction and devolatilisation.

4. Conclusions
A detailed model was developed to simulate the transient flame propagation process in a dust cloud, which is a highly complex system because the gas and solid phases are dynamically, thermally, and chemically coupled. The model includes detailed chemistry for the gas-phase combustion, devolatilisation kinetics, full coupling between the gas and solid phases, and radiative heat transfer. Here are the major conclusions:

(1) The flame-speed oscillation phenomenon, which was observed for carbon-dust clouds in a previous study, was not observed here for coal dusts. The reason is that for nonvolatile dusts, flame propagation is largely controlled by particle-surface reactions. Because a velocity slip exists between the two phases, the particle-number density ahead of the flame front has a periodic change with time. This is equivalent to a change in the local fuel-equivalence ratio and thus causes flame-speed oscillation. For high-volatile dusts such as coal, however, flame propagation is dominated by devolatilisation and the combustion of volatiles. Particle surface reactions have little impact on the flame speed, which essentially depends on the devolatilisation rate. As a result, flame-speed oscillation was not observed for such systems.
(2) The detailed flame structures show that the flame can be divided into five zones: unburned, preheat, devolatilisation, reaction (gas phase), and post-reaction. The reaction zone presents combustion of the volatiles and is typically thin. The devolatilisation zone is wider than the reaction zone because the combustion rate of volatiles is much faster than the devolatilisation rate. The rates of particle surface reactions are much lower than the devolatilisation rate, indicating that volatile combustion is the main contribution of heat release.

(3) Flame speeds increase when particle size decreases. This is because the smaller particles have a larger surface to volume ratio and thus their temperatures can be raised more quickly under the same hot environment. Therefore, the devolatilisation rate of smaller particles is much faster.

References


