Combustion and Flame 198 (2018) 14–23

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Laminar combustion regimes for hybrid mixtures of coal dust with methane gas below the gas lower flammability limit

Chris T. Cloney[a,*], Robert C. Ripley[a,b], Michael J. Pegg[a], Paul R. Amyotte[a]

[a] *Dalhousie University, Process Engineering & Applied Science, Halifax, Canada*
[b] *Lloyd's Register, Applied Technology Group, Halifax, Canada*

ARTICLE INFO

Article history:
Received 13 June 2018
Revised 17 July 2018
Accepted 3 September 2018

Keywords:
Laminar flame propagation
Coal dust
Methane Gas
Hybrid mixtures
Combustion regime diagrams

ABSTRACT

Understanding flame propagation in dust clouds and hybrid mixtures requires knowledge of the fundamental combustion processes and their coupling interaction. The objective of this work is to use computational fluid dynamics to classify laminar flame structure in hybrid mixtures where the initial gas concentration is below the lower flammability limit. Particular focus is given to the role of reaction chemistry and overall equivalence ratio on flame structure and burning velocity. Through this study, five flame regimes were determined: fuel-lean flames (Type I), volatile-lean flames (Type II), volatile-rich flames (Type III), transition flames (Type IV), and kinetic-limited flames (Type V). Gas-phase chemistry was found to play a critical role in burning velocity for Type III, IV, and V flames. Burning velocities at hybrid volatile component equivalence ratios less than 0.9, were found to be less sensitive to reaction kinetics. Further research using this model will focus on initial gas concentrations above the lower flammability limit, exploring the flammability limits of hybrid mixtures, and extending the results to turbulent flames in system geometries relevant to industrial safety.

1. Introduction

Hybrid mixtures of combustible dust and flammable gas represent enhanced industry hazards due to reduced flammability limits and increased flame propagation rates over dust alone [1]. Hybrid mixtures can arise in several industries including mining [2], pharmaceutical [3], and textile manufacturing [4]. Although numerous experiments investigating closed-volume explosion of hybrid mixtures have been reported in the literature (e.g., see [5–10]), limited understanding of the combustion process and coupling mechanisms between the dust and gas has been achieved to date.

The objective of the current investigation is to use computational fluid dynamics (CFD) to explore laminar flame structure in hybrid mixtures where the initial gaseous fuel is present at concentrations below the gas lower flammability limit (LFL). The main focus is on classifying flame structure based on dust concentration and gas concentration. The outcome of this work is a proposed combustion regime diagram for hybrid mixtures under these conditions.

A secondary focus of the current investigation is to explore the impact of gas-phase chemistry on burning velocity and flame structure. For this purpose, parametric analysis is performed with four reaction mechanisms: a single-step global reaction model; a two-step global reaction model; an 84-step semi-detailed kinetics mechanism; and a 325-step full kinetics mechanism.

The CFD model developed by Cloney et al. [11] is used to predict burning velocity and flame structure of hybrid mixtures in this work. In the previous investigation, burning velocity and structure of methane gas flames and coal dust flames were explored using this model. Although simulations were performed that included the four reaction mechanisms, they were only for a mono-size dust cloud with 4 µm particles at a concentration of 144 g/m^3.

In the current investigation the dust concentration is varied between 50 and 1000 g/m^3 for all reaction mechanisms. Furthermore, hybrid simulations are explored using the single-step and two-step reaction models with initial gas concentrations up to an equivalence ratio of 0.5. All simulations were completed with 10 µm coal particles in this work.

The remainder of the current investigation is outlined as follows: Section 2 gives background information on previous development of combustion regime diagrams for hybrid mixtures, and the various equivalence ratios used in this work. Section 3 gives a description of the computational model and example simulation results. Section 4 and Section 5 present predicted burning velocity and flame structure for coal dust alone and for hybrid mixtures, respectively. Lastly, in Section 6 combustion regime diagrams for

---

* Corresponding author.
E-mail address: chris.cloney@dal.ca (C.T. Cloney).

https://doi.org/10.1016/j.combustflame.2018.09.004

hybrid mixtures are developed outlining the flame structure at different dust and gas concentrations, followed by the conclusions of the study.

2. Background

2.1. Combustion regime diagrams

Although regime diagrams have long been used to visualize turbulence and chemistry interaction in premixed and diffusion flames (e.g., see the description of Peters [12]), it was not until the work of Garcia-Agreda et al. [8] that they were discussed in relation to hybrid mixtures of combustible dust and flammable gas. The study of Garcia-Agreda included closed-volume explosion bomb experiments with various mixtures of nicotinic acid (niacin) dust and methane gas. They summarized these results as so-called “explosion regime diagrams”, where maximum rate of pressure rise was plotted on a plane with dust concentration on the ordinate and gas concentration on the abscissa.

Garcia-Agreda et al. [8] divided the regime diagram into five areas based on the concentration of each fuel relative to its lower flammability criteria. The five regimes outlined in their work are as follows: dual-fuel explosion in which both fuels are above their lower flammability criteria; gas-driven explosion in which the gas is above the LFL, but the dust is below the minimum explosible concentration (MEC); dust-driven explosion in which the dust is above the MEC, but the gas is below the LFL; synergistic explosion in which both fuels are below their lower flammability criteria but the mixture still explodes; and non-explosion in which the mixture cannot support flame propagation. The work of Garcia-Agreda et al. [8] was extended by Sanchirico et al. [9] to include mixtures of niacin dust and acetone vapor. Sanchirico et al. [9] also plotted the results of Denkevits [13] for graphite dust and hydrogen gas, and of Pilão et al. [14] for cork dust and methane gas, in terms of explosion regime diagrams.

A recent investigation by Cloney et al. [10] focused on reviewing experimental data available in the literature to further develop hybrid explosion regime diagrams. In this work, 15 previous studies were classified in terms of ignition energy, ignition delay time, dust concentration, and gas concentration.

Cloney et al. [10] proposed that above the gas LFL, gas-only explosion, two-stage explosion, single-stage coupled explosion, and dust-only explosion classifications should be included in regime diagrams, based on the experimental work of Denkevits [13] and Denkevits and Hoess [15]. From analysing the work of Amyotte et al. [16], Khalil [17], Hossain et al. [18], and Ajrash et al. [19], and borrowing from concepts used in the droplet combustion literature (e.g., see Chiu et al. [20] and Nakamura et al. [21]) these authors also proposed group particle combustion and isolated particle combustion below the gas LFL.

In their work, Cloney et al. [10] demonstrated gaps in coverage throughout the dust and gas concentration range, and insufficient experimentation to fully understand the underlying combustion processes. These authors suggested CFD modeling as a viable alternative to further investigate combustion phenomena in hybrid mixtures.

The current study represents the first step in classifying hybrid mixture flame propagation using CFD modeling. It focuses on laminar flow conditions and on hybrid mixtures where the gas concentration is below the LFL. Future investigation will focus on hybrid mixtures where the gas stoichiometry is above the LFL and determining the overall flammability limits of hybrid mixtures. Subsequent work will also focus on extending the results to closed-volume explosion conditions relevant to laboratory testing. This includes the effect of particle size distribution and turbulent combustion on flame propagation. The first of these can be included directly with the Lagrange particle discretization in the computational model described by Cloney et al. [11]. Turbulent flow characteristics and combustion may be included based on the Eddy Dissipation Concept [22] previously used to simulate combustion of pulverized coal by Christ [23] or the Partially Stirred Reactor model previously used to simulate spray combustion with complex chemistry by Nordin [24].

2.2. Equivalence ratios

In this work, several equivalence ratios can be defined for analysing the results. The following sections provide a summary of these equations for methane gas, coal dust, and hybrid mixtures considering reaction of the volatiles alone and volatiles combined with surface reaction. See the work of Cloney [25] for a full derivation of the equivalence ratios used herein.

2.2.1. Methane gas

The gas equivalence ratio is defined as the fuel-to-air ratio of methane gas divided by the stoichiometric fuel-to-air ratio of methane:

$$\Phi_{\mathrm{g}} = \frac{(F/A)^{\mathrm{V}}_{\mathrm{g}}}{(F/A)^{\mathrm{V}}_{\mathrm{St}}} \tag{1}$$

where $(F/A)^{\mathrm{V}}_{\mathrm{g}}$ is the fuel-to-air ratio of methane gas in the mixture and $(F/A)^{\mathrm{V}}_{\mathrm{St}}$ is the stoichiometric fuel-to-air ratio which can be calculated as 0.0582. The fuel-to-air ratio of methane in the mixture can be defined in terms of the mass fractions of methane and air. In a gas mixture containing only these two components, the equivalence ratio can be calculated as:

$$\Phi_{\mathrm{g}} = \frac{17.18 Y_k}{(1 - Y_k)} \tag{2}$$

2.2.2. Coal dust (volatile component)

The coal dust equivalence ratio considering only the volatile component of the fuel is calculated as the fuel-to-air ratio of volatiles from the coal, divided by the stoichiometric fuel-to-air ratio:

$$\Phi^{\mathrm{v}}_{\mathrm{p}} = \frac{(F/A)^{\mathrm{V}}_{\mathrm{p}}}{(F/A)^{\mathrm{V}}_{\mathrm{St}}} \tag{3}$$

where the fuel-to-air ratio of coal is equal to the mass concentration of volatiles divided by the mass concentration of air. In the present work, the dust is assumed to contain 40% volatiles by mass and the volatiles are assumed to contain only methane gas. Assuming ambient pressure of 101,325 Pa and temperature of 300 K, the coal dust equivalence ratio considering only the volatile component of the dust can be calculated as:

$$\Phi^{\mathrm{v}}_{\mathrm{p}} = 5.864 \sigma_{\mathrm{p}} \tag{4}$$

where the dust concentration, σ_{p} must be specified in kg/m^3. Letting $\Phi^{\mathrm{v}}_{\mathrm{p}} = 1$, the stoichiometric concentration of coal dust considering only the volatile component is calculated as 170 g/m^3.

2.2.3. Coal dust (volatile and carbon components)

The coal dust equivalence ratio considering both the volatile and carbon components of the fuel, is calculated as the total fuel-to-air ratio from the dust divided by the total stoichiometric fuel-to-air ratio:

$$\Phi^{\mathrm{t}}_{\mathrm{p}} = \frac{(F/A)^{\mathrm{t}}_{\mathrm{p}}}{(F/A)^{\mathrm{t}}_{\mathrm{St}}} \tag{5}$$

Assuming that the ash and moisture content of the coal is negligible, and that the volatiles contain only methane, the molar ratio of solid carbon to methane in the fuel, $C^{\mathrm{S}}_{\mathrm{p}}/C^{\mathrm{V}}_{\mathrm{p}}$, is calculated as