Effect of Radiation on the Propagation of Planar Coal Dust Flames in Air

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1 Introduction

The structure of flames propagating through suspensions of organic dust depend and on many factors, including volatile content, moisture content, Damkhöler number, Lewis number, particle diameter, and dust concentration. In many cases, the flame structure consists of a preheat zone where conduction transfers energy to the cold gas and radiation from the flame and products transfers energy to the cold fuel particles. After preheating, moisture (water) and fuel begin to evaporate and devolatilize from the organic particles. Eventually the fuel vapor and particles reach ignition, and then competing reactions involving carbon char on the surface of the particles and homogeneous reactions between air and volatiles take place. Ash, unburned fuel particles, and high-temperature CO_2 and H_2O emit radiation, some of which is absorbed in the preheat zone. Details of the flame structure for different dusts vary greatly and the preheat and reaction zones may contain various subzones within them [1].

Experiments of dust flame propagation indicate that the flame speed varies with time [2, 3] and may even pulsate [4]. Lycopodium dust flames [3] initially propagate away from the closed end of a duct at a low velocity, ~ 1 m/s, but can accelerate to ~ 18 m/s. Experimental images show a very broad incandescent region in front of the lycopodium flame, which is an effect likely due to a combination of particle emission and scattering of radiation emitted from the products. Simulations of lycopodium dust flame propagation in this apparatus [3] included the influence of turbulence produced during dust dispersal, but not thermal radiation. Measurements of the radiation intensity from a coal-dust fireball emitted from similar ducts was significant [2].

Radiation is often neglected in modeling due to its inherent complexity and high computational cost, even though it can be the dominant mode of heat transfer to the preheat zone of laminar dust flames [5]. Optically thick diffusion approximations [6] are typically assumed when radiation is considered, even through the product zone may be optically intermediate. More recent simulations used a formal discrete ordinates radiation model [7], but this has only been applied to incompressible calculations.

Creating a suitable approximation to the radiative transfer equation (RTE) that is valid for the wide range of optical thicknesses in dust explosion scenarios is a significant challenge. Consider a layered dust explosion [8]. Regions with dry cold air will be almost transparent and approach the photon freestreaming limit. Regions where the dust is burning will range from optically intermediate to optically thick, depending on particle concentration, pressure, etc. Regions near a source of dust, such as a dust



Figure 1: Diagram of the computational domain and initial conditions.

layer, will be optically very thick and approach the diffusion limit. Many radiation models work in either optically thick or optically thin regions, but usually not both. Traditional elliptic spherical harmonics approximations (P_N), such as P_1 , become singular in the free-streaming limit. Discrete-ordinate methods have difficulty converging in media that is both optically thick and scattering [9]. Filtered spherical harmonic approximations (FP_N) [10, 11] that are accurate in optically thin and thick regions have been recently developed. FP_N approximations are hyperbolic and have solution algorithms that are similar to TVD-based methods for traditional gas-dynamic calculations. This makes coupling radiation transport to compressible reacting flow far simpler than traditional elliptic P_N or discrete ordinates approximations.

In this work we explore the effect of radiation on the ignition and propagation of planar (1D) flames through coal dust and air mixtures. Third-order filtered spherical harmonics (FP_3) is used to model radiation. Closed and open ducts are considered.

2 Numerical Model and Computational Setup

The governing equations apply an Eulerian approach for the both gas and granular (coal) phases in one-dimension [8]. This model has been shown to work well for simulating shock propagation in dust, granular shocks, lifting of dust layers, etc. The governing equations are solved using a high-order Godunov approach. Details of the model, numerical solution procedure, treatment of non-conservative terms, and test cases can be found in [12].

The coal particles are assumed to be Illinois coal with 16.15% moisture, 42.59% volatiles (approximated as CH₄), 40.23% carbon char, and 1.03% ash [7]. The initial density and diameter of the particles was 1,200 kg/m³ and 30 μ m, respectively. Arrhenius expressions are used to describe the rates of moisture evaporation [13], CH₄ devolatilization [14], and combustion of carbon char [15]. For the char reaction a linearized one-film model [16] is used to estimate the oxygen mass fraction at the surface of the coal particles. The four-step Jones-Lindstedt mechanism [17] was used to describe gas-phase reactions between CH₄, O₂, CO₂, CO, H₂O, and H₂.

Radiation is assumed to be gray and is modeled using the FP₃ approximation to the RTE. The resulting equations are solved using a third-order TVD approach with the Rusanov Riemann solver [18]. Scattering is assumed to be isotropic. The Buckius and Hwang correlation [19] is used to compute the Planck-mean extinction and scattering coefficients for the coal dust. The Planck-mean absorption coefficients for CO₂, CO, CH₄, and H₂O were taken from [20].

The computational domain and initial condition are shown in Fig. 1. Two cases are considered, (1) a freely propagating flame from the close end of a tube with one open end and (2) flame propagation in a completely closed vessel. The domain length for the freely propagating flame case is 2 m and is discretized with 6000 cells (\sim 11 particle diameters). The closed vessel case is 42.5 cm in length (discretized with 1500 cells or about 9.4 particle diameters) and contains two 20 cm-long chambers separated by an insulating and transparent window 2.5 cm in width. The window blocks convective and conductive heat transfer between the chambers, but allows radiation generated by the combustion products and ash in the first chamber to heat particles in the second chamber. Two initial particle volume



Figure 2: Effects of radiation and initial equivalence ratio, ϕ , on (a) flame position and (b) the absolute flame velocity as a function of time.

fractions were considered, 0.01% and 0.02%, with corresponding equivalence ratios of $\phi = 1.2$ and 2.4. The flame was ignited by setting the initial temperature of the coal dust to 1000 K and the air to 1500 K for the first 2 cm of the domain. The left and right boundaries were assumed to be cold and black.

3 Results and Discussion

The flame position and speed as a function of time for the open tube are shown in Fig. 2. The flame speed is relatively low for a while and then accelerates rapidly to about 16 m/s and 5 m/s in the $\phi = 1.2$ and $\phi = 2.4$ cases, respectively. This acceleration is qualitatively similar to experiments [2, 3]. The total absorption coefficient in the products is about 1 m⁻¹ and 4 m⁻¹ for the $\phi = 1.2$ and $\phi = 2.4$ cases, respectively. The product region is optically thin when it is close (~10 cm) to the left radiatively absorbing boundary. (The flame can "see" the left boundary.) As a result, emission losses from the flame that exit through the left boundary are initially large. The product region becomes optically thicker as the flame propagates into the tube, and more radiative energy is transferred to the preheat zone. The incident radiation, defined by

$$G = \int_{4\pi} I d\Omega, \tag{1}$$

where I is the radiation intensity and Ω is the solid angle, builds in strength as the flame propagates (see Fig. 3.) The increase of incident radiation means that particles in the preheat zone are heated faster. (The radiation heat sources are given by

$$-\nabla \cdot \mathbf{q}_{\text{rad}} = \kappa (G - 4\pi I_b) \tag{2}$$

where κ is the absorption coefficient, \mathbf{q}_{rad} is the radiative heat flux, and I_b is the blackbody intensity.)

In the early stages of flame propagation conduction is the primary mode of heat transfer to the preheat zone which is consistent with [7]. At later times, radiative heat transfer to the particles becomes an order of magnitude larger than conduction as the incident radiation of the products increases (see Fig. 3).



Figure 3: Flame structure at 395 ms and 574 ms for the $\phi = 1.2$ case (a) gas- and solid-phase temperature (T_{gas} and T_{coal} , respectively) and incident radiation and (b) source term strengths to the internal energy equations due to conduction for the gas-phase and radiative heat transfer to the solid and gas-phases.

The results for the two-chamber closed geometry are shown in Figs. 4 and 5. Similar to the open-ended tube cases, the flame initially propagates slowly due to radiative heat losses. It then accelerates as the incident radiation builds and eventually approaches the transparent window. Radiative heat from products in the left chamber is transferred through the window to particles in the right chamber. Eventually dust in the right chamber ignites. The speed of the flame in the right chamber is much faster after ignition than in the left chamber due to higher incident radiation and larger optical depth of the products. The flame propagates through the right chamber in ~ 20 ms for $\phi = 1.2$ and ~ 90 ms for the $\phi = 2.4$ in comparison to ~ 300 ms it took for the flame to propagate through the left chamber in both cases.

4 Conclusions

Numerical simulations of one-dimensional coal-dust flames in air with $\phi = 1.2$ and $\phi = 2.4$ were conducted to evaluate the influence of thermal radiation on ignition and flame propagation. Radiative energy was assumed to be gray and was modeled with a third-order filtered spherical harmonics approximation to the radiative transfer equation. Two geometrical configurations were considered, flame propagation in an open tube and flame propagation in an enclosed tube with two-chambers separated by a transparent window. The results indicate that radiation has a significant effect on the acceleration of the flame for both dust concentrations. Furthermore, radiative heat transfer was significant enough to ignite particles on the opposite side of a transparent window. These results confirm that radiative heat transfer can have significant and even dominant effect on flame propagation through dust suspensions. The degree of this importance is likely influenced by particular details of type of coal dust, selected combustion models, dust concentration, and approximation used to estimate optical properties. Examining the sensitivity of our model to such parameters is a topic of future work.

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Figure 4: Computed results for the two-chamber case with $\phi = 1.2$ showing (a) the particle temperature and (b) the incident radiation as a function of time. The transparent window separating the two chambers is indicated by the blue rectangle. Time (ms) is noted on each curve.



Figure 5: Computed results for the two-chamber case with $\phi = 2.4$ showing (a) the particle temperature and (b) the incident radiation as a function of time. The transparent window is indicated by the blue rectangle. Time (ms) is noted on each curve. The particle temperature in the left chamber is not shown at times greater than 349 ms and is shown only near the flame at times of 201, 247, and 338 ms for clarity.

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References

- [1] Bidabadi, M., Dizaji, F., Dizaji, H., and Ghahsareh, M., J. of Cent. South Univ., Vol. 21, No. 1, 2014, pp. 326–337.
- [2] Cao, W., Gao, W., Liang, J., Xu, S., and Pan, F., J. Loss Prevent. Proc., Vol. 29, No. 0, 2014, pp. 65–71.
- [3] Spijker, C., Kern, H., and Raupenstrauch, H., "A CFD Approach for Dust Explosions Based on OpenFOAM," *Proceedings of the Tenth International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosions (X-ISHPMIE)*, edited by T. Skjold, R. K. Eckhoff, and K. van Windergerden, 2014.
- [4] Hanai, H., Maruta, K., Kobayashi, H., and Niioka, T., P. Combust. Inst., Vol. 27, No. 2, 1998, pp. 2675–2681.
- [5] Deshaies, B. and Joulin, G., SIAM J. Appl. Math., Vol. 46, No. 4.
- [6] Slezak, S. E., Buckius, R. O., and Krier, H., Combust. Flame, Vol. 59, No. 3, 1985, pp. 251–265.
- [7] Qiao, L. and Xu, J., Combust. Theor. Model., Vol. 16, No. 5, 2012, pp. 747–773.
- [8] Houim, R. W. and Oran, E. S., P. Combust. Inst., Vol. 35, 2014.
- [9] Modest, M. F., Radiation Heat Transfer, Academic Press, 3rd ed., 2013.
- [10] McClarren, R. G. and Hauck, C. D., *Journal of Computational Physics*, Vol. 229, No. 16, 2010, pp. 5597–5614.
- [11] Radice, D., Abdikamalov, E., Rezzolla, L., and Ott, C. D., "A new spherical harmonics scheme for multi-dimensional radiation transport I. Static matter configurations," *J. of Comput. Phys.*, Vol. 242, No. 0, 2013, pp. 648–669.
- [12] Houim, R. W. and Oran, E. S., http://arxiv.org/abs/1312.1290v2, 2013.
- [13] Bradley, D., Lawes, M., Park, H.-Y., and Usta, N., Combust. Flame, Vol. 144, 2006, pp. 190 –204.
- [14] Govind, R. and Shah, J., AIChE Journal, Vol. 30, No. 1, 1984, pp. 79–92.
- [15] Baek, S. W., Sichel, M., and Kauffman, C. W., Combust. Flame, Vol. 81, No. 3, 1990, pp. 219–228.
- [16] Turns, S. R., An Introduction to Combustion: Concepts and Applications, McGraw-Hill, 2nd ed., 2000.
- [17] Jones, W. and Lindstedt, R., Combust. Flame, Vol. 73, No. 3, 1988, pp. 233 249.
- [18] Rusanov, V. V., J. Comput. Math. Phys., Vol. 1, 1961, pp. 267–279.
- [19] Buckius, R. O. and Hwang, D. C., J. Heat Trans., Vol. 102, No. 1, 1980, pp. 99–103.
- [20] "International Workshop on the Measurement and Computation of Turbulent Nonpremixed Flames," http://www.ca.sandia.gov/TNF/radiation.html, 2003, Accessed: Sept. 21, 2014.