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A reaction engineering approach to modeling dust explosions

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HIGHLIGHTS

- We present a two-scale reaction engineering model for dust explosions.
- Particle scale model incorporating transport effects and kinetics is presented.
- Quasi-homogeneous (dust-) cloud scale CFD model linked to particle-scale model.
- Model validated for aluminum (metallic) and starch (organic) dust explosions.
- Presented case study demonstrates applicability to real situations.

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ABSTRACT

Dust explosions are a major hazard frequently encountered in vital sectors like food, energy, defense (propellants and explosives) and pharmaceuticals. These explosions emanate from rapid combustion of clouds of suspended fine particles in the micron range. Quantitative estimation of dust explosion propagation is crucial to their mitigation, and for providing estimates of physical quantities that determine the explosion behavior for design of safety systems. In this contribution, a multi-scale reaction engineering approach for modeling dust explosions has been presented. In the model, two scales are considered. At the particle scale, a detailed model involving various transport steps is written and solved for a variety of different boundary conditions. This model is used to build an effective reaction rate term which is incorporated in the dust cloud-scale CFD model through an appropriate source term. The CFD model for the effective dust cloud mixture is then executed to model the propagation of the dust explosion. Validation of the developed CFD model has been carried out for two different kinds of dust particles, aluminum (metallic dust) and starch (organic dust), for experimental data published in literature. Finally, a case study has been presented which shows the applicability of present approach in modeling real situations. It is demonstrated that using the same physics and estimated kinetic parameters from particle scale model or smaller scale experiments, fairly satisfactory prediction for dust explosions in real geometries could be obtained.

1. Introduction

Dust explosions involve rapid combustion of fine, combustible dust particles (generally in the micron size range). Following this rapid combustion, typically the pressure of product gases, in the enclosure containing the dust-oxidizer mixture, increases many folds within a fraction of second. This causes the "explosion" and can potentially cause collapse of the enclosure itself, or lead to secondary dust explosions which could be equally damaging to life and property even at some distance from the original point of the explosion. Historically the first recorded incidence of a dust explosion was at an Italian flourmill in 1785, although it was almost certainly not the first to occur [1]. These hazards are frequently encountered in vital industries and sectors of a country including agriculture, food processing, coal mining, defense (involving solid, granular explosives and propellants), plastic, wood and other materials processing, and pharmaceuticals. In these industries, various unit operations like storage, grinding, transportation and pneumatic conveying are susceptible to dust explosion hazards. Several excellent texts are now available which provide excellent reviews of this important but relatively less studied safety hazard (for example, see the works of Eckhoff [1], Field [2], Palmer [3] and Field [4]). However, most of these books deal with dust explosion as a safety and hazard issue, discuss ways of mitigating and preventing these, but few treat the underlying physics in great detail.

Proper understanding of dust explosion phenomena is necessary for design of any preventive or protective system to prevent

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such hazards causing accidents. Since the explosions result in rapid pressure build-up and heat localization, it is crucial to estimate the (primarily convective) transport rates with accuracy, so that a protection system could be designed and safety protocols may be established. This is of particular relevance since experiments are difficult to perform in these situations, and investigations leading to quantitative estimates can only be performed in well-designed, small-scale laboratory units, such as the classical Siwek 20L apparatus (e.g. [5]). Dust explosion experiments in actual process plants are rarely performed, due to the prohibitively high cost and risk involved ([6] is a notable exception).

Extensive work on modeling dust explosions using CFD [7–9] in conjunction with input from laboratory scale experiments [10–12] has revealed that much more work is needed on the basic physics and chemistry. Ogle [13] was perhaps the first one to emphasize the need of dust explosion prediction using material properties of the explosible mixture. Ogle [13] has developed a model for simulation of aluminum/air explosions in closed vessel, assuming spatially uniform pressure at any instant. Relation between particle scale surface burning rate and volumetric reaction rate at cloud scale was shown. However in this work particle scale modeling was not attempted and surface reaction rate was assumed as rate controlling mechanism for aluminum particle combustion. Further, 20 L spherical vessel was assumed as batch reactor for dust explosion reaction modeling. These simplified assumptions (may be due to lack of computational power) resulted in disagreement between Ogle's [13] theoretical and experimental work. Nevertheless this work suggested an important methodology based on material properties of combustible mixture and cloud scale hydrodynamics for dust explosion prediction.

This contribution was motivated by the fact that proper understanding of dust explosion phenomenon is necessary at "particle scale" as well as at "cloud scale". "Particle scale" deals with mechanism of ignition, gas–solid non-catalytic reaction, all at the size or length scale of the dust particles (which is usually a few microns). The transport phenomena at the "cloud scale" deals with flame and pressure propagation, which is actually in a two-phase gas–solids mixture (referred to as the "cloud"), even though for many purposes it may behave like a pure gas cloud. This overall vision of the dust explosion mechanism is reflected schematically in Fig. 1. This understanding and distinction of scale-wise transport should lead us to the formulation of a mathematical model to relate factors, parameters and design variables. When coupled with computational fluid dynamics (such as the work of Skjold et al. [8]), it is possible to translate the particle-scale and cloud-scale physics to complex geometries.

In an earlier contribution [14], a CFD model has been presented in which the dust-air mixture is viewed as an effective gas, and the explosion was driven by an effective source term resulting from particle-scale combustion. In this contribution, we present the combined model (involving particle-scale combustion and cloud-scale transport), show validation of this model and extend it to model a case study. Even with the assumption of quasi-homogeneous dust cloud, the simulation for dust explosion in industrial size of vessel $\sim$10.3 m^3 presented in proposed manuscript takes considerable time of the order of month with IBM Server: 64 bit Operating System, Processor Intel(R) Xenon (R) CPU, 2.27 GHz, 4.0 GB Memory. This is due to the fact that the time step used in proposed simulation is $\sim 10^{-5}$ s where as total time of combustion in the vessel is of the order of $\sim$1.0 s. The main advantage of proposed model compared with existing models is that it is based on material properties of fuel and oxidizer at particle scale and at cloud scale CFD could be applied which will make it more generalized and with lesser assumptions compared to existing models. This will also lead to fundamental understanding of dust explosion phenomenon. This model is versatile and could be applied for any geometry.

2. Representing particle scale phenomena in dust cloud CFD

From our presentation of Fig. 1, it is clear that we intend to develop an "effective" description of particle scale phenomena and then connect it to the cloud scale CFD model. Descriptions at particle scale can be analytical, numerical or empirical (through correlations). Either of these descriptions are sensitive to the nature of the dust particles, the oxidizers, and most importantly, the average inter-particle distance in the cloud. This factor actually determines the kind of combustion the dust particles would exhibit, and hence what role it would have in determining the overall explosion behavior.

If these particles are separated by a large distance, single particle combustion will define the combustion behavior of the cloud. However if the concentration of dust particle is high and particles are in the vicinity, then the so-called *Group Combustion* or *Cloud Combustion* modes is observed [15]. Therefore, the average inter-particle distance is an important factor in defining the cloud scale dust explosion phenomenon.

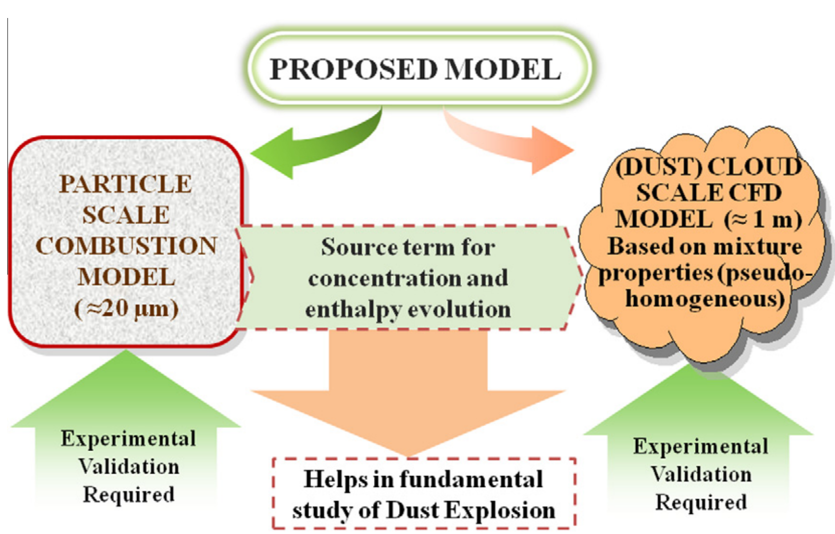

Fig. 1. Proposed multi-scale approach for dust explosion modeling.