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Simulating the Influence of Obstacles on Accelerating Dust and Gas Flames

T. Skjold ^{1,2}, Y.K. Pu³, B.J. Arntzen², O.R. Hansen¹, I.E. Storvik¹, O.J. Taraldset^{1,2} and R.K. Eckhoff²

¹GexCon AS, Fantoftveien 38, 5892 Bergen, Norway

² University of Bergen, Department of Physics and Technology, Bergen, Norway ³ National Microgravity Laboratory, Institute of Mechanics, Chinese Academy of Sciences, Beijing, China

Corresponding author, T. Skjold: trygve@gexcon.com

1 Introduction

A new CFD-code called DESC is currently being developed for predicting flow, flame propagation and pressure build-up during dust explosions in complex geometries. Combustion models in the first versions of DESC will use similar correlations for turbulent burning velocity as the CFD-code FLACS for gas explosions. The main aim of the present work is to test the chosen approach by comparing experimental results on the influence of obstacles on flame propagation in cornstarch-air and methane-air mixtures, to results obtained with DESC and FLACS for the same mixtures.

2 Experiments

The experimental work on the influence of obstacles on flame propagation is described by Pu (1988) and Pu *et al.* (1988); it was performed in a closed vertical tube, illustrated in Figure 1. These experiments are well suited for comparison with CFD-codes for several reasons: dust and gas explosions were initiated from the same initial flow conditions, the dispersion system is described in detail, including turbulence and pressures during the dispersion process, flame arrival times and pressure in the tube were measured simultaneously, and both tests with and without obstacles were included. Figure 2 indicate that the flame propagates faster in a lean mixture of 6.2 % methane in air, than through a 550 g m⁻³ cornstarch-air cloud, especially during the initial phase of the explosion.

3 Simulations

In the present version of DESC (version 1.0b2), the dispersed dust particles are assumed to be in dynamic and thermal equilibrium with the gaseous phase. This corresponds to the Eulerian approach in the limiting case when the Stokes number approaches zero, so-called equilibrium mixture (Crowe *et al.*, 1998). It is further assumed that the reactants have known chemical composition, and that product composition can be estimated through simplified chemical equilibrium calculations. Laminar burning velocities are found by applying an inverse correlation to turbulent burning velocities estimated from pressure-time curves obtained in standardized 20litre explosion vessels (Skjold *et al.*, 2005a; Skjold *et al.*, 2005b), and the fraction of dust that is allowed to react is estimated from heats of combustion and experimentally determined explosion pressures. In both FLACS and DESC, the flame is described by the so-called β flame model, in which the flame thickness depends on the size of the grid cells (Arntzen, 1998). Heat loss by both convection and radiation is accounted for in the simulations. The empirical model used for the DESC simulations in this work is based on experiments with two types of cornstarch in a 20-litre vessel at the University of Bergen (Skjold *et al.*, 2005; Skjold, 2003); experimental results and empirical model are summarized in figures 3 and 4. Note that the cornstarch used to generate the empirical model had K_{st} values close to 150 bar m s⁻¹; this value may deviate somewhat from the cornstarch used by Pu. According to Beck *et al.* (1997), K_{st} values for cornstarch are typically between 100 and 200 bar m s⁻¹. However, Pu determined the average particle size of the cornstarch to 14.7 µm (standard deviation 5.1 µm) by direct imaging, which is quite similar to the starch used in this work (standard percentile readings determined by laser diffraction, for both types of maize starch, were about 6, 13 and 20 µm for the 10, 50 and 90 percentiles, respectively).

The initial conditions used in the simulations assumed a homogeneous dust cloud with an integral length scale of 1 cm, and root-mean-square of turbulence fluctuations equal to 20 cm s⁻¹; this should be comparable to the values measured by Pu (1988) for an ignition delay time of 300 ms.

4 Results

Simulated and experimental results are compared in Figure 6. The effect of the obstacles on flame propagation and pressure build-up is evident for both types of fuel. The size of the grid cells also influences the results, especially for the coarsest of the three grids (28.5 cm cubical grid cells).

Although the initial pressure rise is somewhat delayed in the simulations, compared to experimental results, the results obtained with FLACS, for mixtures of 6.2 % methane in air, are quite similar to the experimental results presented by Pu (1988). However, the results obtained with DESC for 550 g m⁻³ cornstarch-air mixtures are significantly different from the experimental results; in the simulation, the flame propagates much faster than in the experiment, and even faster than the simulated flame in the methane-air mixture (contradicting the results in Figure 2).

5 Discussion

The positive feedback mechanism between turbulence and combustion results in strong acceleration of the flame in the central part of the tube. Hence, the results are sensitive to how well the initial part of flame propagation can be modelled. In both FLACS and DESC, initial flame propagation is controlled by a sub-grid model. Figure 5 illustrates how the size of the grid cells influences flame propagation in the initial phase; this effect may however be of limited practical significance, since it merely represents a short delay in the development of the explosion.

There can be several reasons for the significant discrepancies between simulated and experimental results for cornstarch. First, the reactivity (e.g. the K_{st} value) of the starch used by Pu may have been somewhat lower than the reactivity of the samples used to generate the empirical model for DESC. Second, combustion of dust-air clouds is characterized by a higher degree of volumetric energy release, compared to premixed gaseous flames (Lee *et al.*, 1987); hence, flame thickness can be expected to have strong influence of on pressure-time curves from dust explosions in closed vessels (Dahoe, 1996). Third, dust flames are probably more non-adiabatic than gaseous flames (Lee, 1988); hence, they may be more influenced by heat loss to walls in small-scale experiments. Finally, the correlations used to estimate turbulent burning velocities for cornstarch-air mixtures may differ significantly from those applicable to gaseous fuels; this is also indicated by results presented by Skjold *et al.* (2005b).

6 Conclusion

It was possible to reproduce the experimental results for lean methane-air mixtures reasonably well with the CFD-code FLACS; hence, similar results for various types of dust may become very useful for DESC validation in the future. However, it is essential that representative experimental data should be used when generating input to the code.

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Figure 1 Schematic diagram of apparatus for explosion tests, from Pu et al. (1988). The closed tube is 0.19 meters in diameter and 1.86 meters long. It is filled with ring-shaped obstacles, and equipped with a piezoelectric pressure transducer and ionisation probes for measuring flame arrival. The ignition source was 0.6 grams of black powder, with total energy release about 1.75 kJ in 25 ms.



Figure 2 Pressure rise and location of flame front as functions of time in 1.86 meter closed tube for mixtures of 6.2 % methane in air and 550 g/m^3 cornstarch in air (from Pu, 1988).



Figure 3 Experimental results for two types of dried cornstarch: **a**) corrected explosion pressure, **b**) size-normalized rate of pressure rise (maximum value corresponding to a K_{st} -value of about 150 bar m/s), and **c**) estimated laminar burning velocities.



Figure 4 Laminar burning velocity and fraction of burnable fuel used as input to DESC; lower flammability limit estimated to 60 g/m³, upper flammability limit arbitrary set to 2000 g/m³.



Figure 5 Vertical cross-section of simulated pipe, illustrating grid cells and simulated flame development for various grids during a cornstarch-air explosion. Flames are plotted as mass fraction of combustion products at various time-steps: after 68 ms, when the flames reaches the first obstruction, and 14 ms after the flames reached the first obstruction. The modelled cornstarch had a K_{st} value of about 150 bar m/s.



Figure 6 Experimental (above) and simulated (below) pressure rise and location of flame front as function of time for flame propagation with and without obstacles in 6.2 % methane-air (left, FLACS simulations) and 550 g/m³ cornstarch-air mixtures (right, DESC simulations) at an ignition delay time of 319 ms; experimental results from Pu (1988). The legend below the plots applies to the simulated data.