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Simulation of dust explosions in complex geometries with experimental input from standardized tests

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Abstract

The present paper describes the development of a new CFD-code (DESC) for the assessment of accidental hazards arising from dust explosions in complex geometries. The approach followed entails the estimation of the laminar burning velocity of dust clouds from standardized laboratory-scale tests, and its subsequent use as input to the combustion model incorporated in DESC. The methodology used to obtain the laminar burning velocities is demonstrated by igniting turbulent propane-air mixtures to deflagration in a standard 20-litre USBM-vessel, and extracting the laminar burning velocity from the pressure–time curves; the results are compared with literature data. Laminar burning velocities for clouds of maize starch dust in air were estimated following the same procedure, and the resulting empirical model was used to simulate dust explosions in a 236-m^3 silo.

Keywords: DESC; Dust explosion; Modelling

1. Introduction

Since many materials that are virtually non-flammable in bulk can become explosive when dispersed in air as fine powder, dust explosions represent a hazard to both personnel and equipment in industries that handle combustible dusts. Although primarily one seeks to prevent accidental dust explosions from taking place, mitigating measures have to be implemented in many situations. Traditionally, the reactivity of explosive dust clouds has been characterized by the rate of pressure rise determined in constant volume explosion vessels, and dimensioning of mitigating measures has relied on empirical or analytical correlations involving parameters such as the K_{St} value. Although such methods may provide acceptable levels of risk in many situations, realistic prediction of flow, flame propagation and pressure build-up during dust explosions in complex geometries can only be accomplished by computational fluid dynamics (CFD). If turbulent combustion of dust clouds can be modelled with sufficient accuracy, design solutions based on CFD will have a much higher potential for being optimised with respect to risk versus cost, compared to solutions based on currently used methods. A recent review of previous work on dust explosion modelling is given by Eckhoff (2003), and some contributions using an approach similar to the one described in the present work is summarized by Skjold et al. (2005).

Since there are many types of combustible dusts, and many parameters influencing the reactivity of each type, it would be a great advantage to be able to extract fundamental flame propagation parameters from results obtained in laboratory tests. The present work explores the possibility of using results from standardized tests in 20-litre explosion vessels as input to the combustion models in an early version of the CFD-code DESC (Dust Explosion Simulation Code).

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2. The DESC project

The main aim of the DESC project is to produce a CFD-code that can estimate the course of industrial dust

explosions; ideally, it should also be possible to simulate the effect of most kinds of mitigation devices such as venting, suppression and explosion isolation. The project involves experimental work, measurements in real process plants, modelling and validation, and is organized as a consortium consisting of the following participants: HSL, GexCon, TNO, Inburex, FSA, Fraunhofer-ICT, Øresund Safety Advisors, Hahn & Co, Lyckeby Culinar and Technical University of Warsaw. Contributions are also received from Fike, Ineris, University of Bergen and Technical University of Delft. Three types of dust are investigated experimentally in the DESC project: coal, potato starch and silicon. However, much of the initial modelling work has been done for maize starch.

3. Modelling

This section describes the present combustion modelling in DESC, which implies that a rough estimate for the laminar burning velocity is found from measured pressure-time curves in a 20-litre vessel. This method is then applied to experimental data for both propane-air mixtures and maize starch-air suspensions, in order to generate input to the combustion model in DESC.

3.1. Modelling in FLACS

DESC is based on the existing FLACS-code for gas explosion modelling. The combustion models in both FLACS and DESC consist of a flame model and a burning velocity model. The flame model controls the localization and area of the flame; the so-called β-model (Arntzen, 1998) is currently used. The burning velocity model determines the velocity of the flame relative to premixed reactants (S_u) by an expression on the form:

$$S_\mathrm{u} = \max(S_\mathrm{QL}, S_\mathrm{T}) \tag{1}$$

where S_QL and S_T are the quasi-laminar and turbulent burning velocity, respectively. The quasi-laminar burning velocity is a correction of the laminar burning velocity S_L, taking into account effects such as flame radius and wrinkling of the flame. The turbulent burning velocity is based on experimental data (Abdel-Gayed, Bradley, & Lawes, 1987) summarized in a correlation by Bray (1990):

$$S_\mathrm{T} = 0.875 \cdot u'_\mathrm{rms} \cdot K^{-0.392} \tag{2}$$

where u'_rms is the root-mean-square of the turbulent velocity fluctuations and K is the Karlovitz flame stretch factor. In FLACS, S_T is found from the equation system:

$$S_\mathrm{T} = \min \begin{cases} S_\mathrm{T1} = 0.96 \cdot S_\mathrm{L}^{0.284} \cdot u'^{0.912} \cdot \ell_m^{0.196} \cdot \nu^{-0.196} + S_\mathrm{L} \\ S_\mathrm{T2} = 1.8 \cdot S_\mathrm{L}^{0.784} \cdot u'^{0.412} \cdot \ell_m^{0.196} \cdot \nu^{-0.196} \\ S_\mathrm{T3} = 3 \cdot S_\mathrm{L}^{4/3} \cdot \ell_m^{1/3} \cdot \nu^{-1/3} \end{cases} \tag{3}$$

where $\ell_m = C_\mu^{0.75} k^{1.5} \varepsilon^{-1}$ is a turbulent mixing length from the k-ε model by Lauder and Spalding (1974), $C_\mu = 0.09$, k is turbulent kinetic energy, ε is dissipation rate of turbulent energy, ν is kinematic viscosity, and S_{T1}, S_{T2} and S_{T3} are expressions for turbulent burning velocity used for low, medium and high turbulence levels, respectively (Popat et al., 1996; Arntzen, 1998).

3.2. Modelling in DESC

In the present version of DESC (version 1.0b2), it is assumed that the dispersed dust particles are 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, Sommerfeld, & Tsuji, 1998). It is further assumed that the reactants have known chemical composition, and that product composition can be estimated through simplified chemical equilibrium calculations. The fraction of dust that is allowed to react (λ) is then estimated from the heat of combustion and experimentally determined explosion pressures.

Since the laminar burning velocity of dust-air suspensions is required by the burning velocity model, S_L is estimated from pressure-time histories measured in standardized 20-litre explosion vessel tests. First, a thin-flame model (Dahoe, Zavenbergen, Lemkowitz, & Scarlett, 1996) is used to estimate the turbulent burning velocity:

$$S_\mathrm{T}(t_{ip}) = \frac{1}{3(p_m - p_i)} \left(\frac{\mathrm{d}p}{\mathrm{d}t}\right)_m \left(\frac{3V_v}{4\pi}\right)^{1/3} \left(\frac{p(t_{ip})}{p_i}\right)^{-1/\gamma} \times \left\{1 - \left(\frac{p_m - p(t_{ip})}{p_m - p_i}\right)\left(\frac{p(t_{ip})}{p_i}\right)^{-1/\gamma}\right\}^{-2/3} \tag{4}$$

where t_{ip} and $p(t_{ip})$ defines the inflection point where the maximum rate of pressure rise $(\mathrm{d}p/\mathrm{d}t)_m$ is determined, p_i is initial absolute pressure, p_m is corrected absolute explosion pressure, and V_v is the volume of the vessel. Second, turbulent flow parameters in the unburned mixture ahead of the flame are estimated. Based on simulations (Skjold, 2003), the turbulent length scale $\ell_\mathrm{LT} = C_\mu k^{1.5} \varepsilon^{-1}$ used in FLACS is assumed equal to 0.006 m. The root-mean-square of the turbulent velocity fluctuations is estimated from a decay law for turbulence in a 20-litre sphere fitted with the rebound nozzle (Dahoe et al., 2001):

$$\frac{u'_\mathrm{rms}(t_{ip})}{u'_\mathrm{rms}(t_0)} = \left(\frac{t_{ip}}{t_0}\right)^n \quad 60\ \mathrm{ms} < t_{ip} < 200\ \mathrm{ms} \tag{5}$$

where $u'_\mathrm{rms}(t_0) = 3.75\ \mathrm{ms}^{-1}$, $t_0 = 60$ ms and $n = -161$.

Lastly, it is assumed that turbulent burning velocities for dust clouds can be estimated from equation system (3), i.e. the same correlations that are used for gas explosions in the FLACS code. Laminar burning velocities are then estimated with an inverse version of system (3):

$$S_{\mathrm{L}} = \max\begin{cases} S_{\mathrm{L1}} = 0.0316 \cdot S_{\mathrm{T}}^{1.279}(t_{ip}) \cdot \ell_{\mathrm{LT}}^{-0.25}(t_{ip}) \cdot u_{\mathrm{rms}}'^{-0.526}(t_{ip}) \\ S_{\mathrm{L2}} = 0.0294 \cdot S_{\mathrm{T}}^{0.75}(t_{ip}) \cdot \ell_{\mathrm{LT}}^{-0.25}(t_{ip}) \end{cases} \tag{6}$$

where a constant value of 1.5×10^{-5} m^2 s^{-1} has been used for the kinematic viscosity of air.

3.3. Propane-air mixtures

In order to test the method outlined in the previous section, laminar burning velocities were estimated for propane-air mixtures from experimental data (Skjold, 2003). The experiments were performed in a 20-litre USBM vessel fitted with a dust dispersion system of the same kind as the one used with the Siwek sphere (Cesana & Siwek, 2001). The correct mixture composition was obtained by first evacuating the 20-litre vessel to, e.g. 0.300 bar absolute, admitting the required amount of propane, admitting additional air to get 0.400 bar absolute, and finally injecting compressed air (20.0 bars gauge) from a 0.60-litre reservoir into the evacuated vessel. The ignition source was an electric arc that could be triggered after a certain ignition delay time (t_v), producing a total energy release of about 6 J in 3 ms. For tests at quiescent conditions, ignition was postponed to several minutes after the injection period was over.

Experimental results and estimated laminar burning velocities are shown in Fig. 1 for various ignition delay times. The significant difference in explosion pressures for quiescent and turbulent conditions when the propane concentrations is higher than about 6 per cent, even for very long ignition delays, is probably due to mainly upwards flame propagation in the quiescent case (Cashdollar et al., 2000). The even spread of estimated laminar burning velocities for propane-air mixtures, for various ignition delay times, around the fitted curve in Fig. 1c, indicates that the effect of turbulence has been more or less filtered out.

In Fig. 2, the fitted curve from Fig. 1c is compared to literature data for the laminar burning velocity of propane-air mixtures (Law, 1993; Vagelopoulos, Egolfopoulos, & Law, 1996; Gibbs, & Calcote, 1959; Metghalchi, & Keck, 1980). Although the estimated laminar burning velocities for concentrations close to stoichiometric are somewhat lower than values found in literature, the results provide a reasonably good estimate in the case of propane-air mixtures.

3.4. Maize starch-air suspensions

Two types of maize starch were used to generate empirical input to the combustion model in DESC: *Meritena A* is from the same lot used by Eckhoff, Fuhre, and Pedersen (1985, 1987), and *Maizena* is a similar product. The particle size distributions were determined by laser diffraction with a Malvern Mastersizer X; standard percentile readings for both types of maize starch were about 6, 13 and 20 μm for the 10, 50 and 90 percentile, respectively. Fig. 3 illustrates some representative particles. Experimental procedures were practically the same as described for propane-air mixtures; however, the appropriate amount of dust was added to the reservoir prior to injection. In one of the test series with Meritena A, two 5 kJ chemical igniters were used as ignition source.

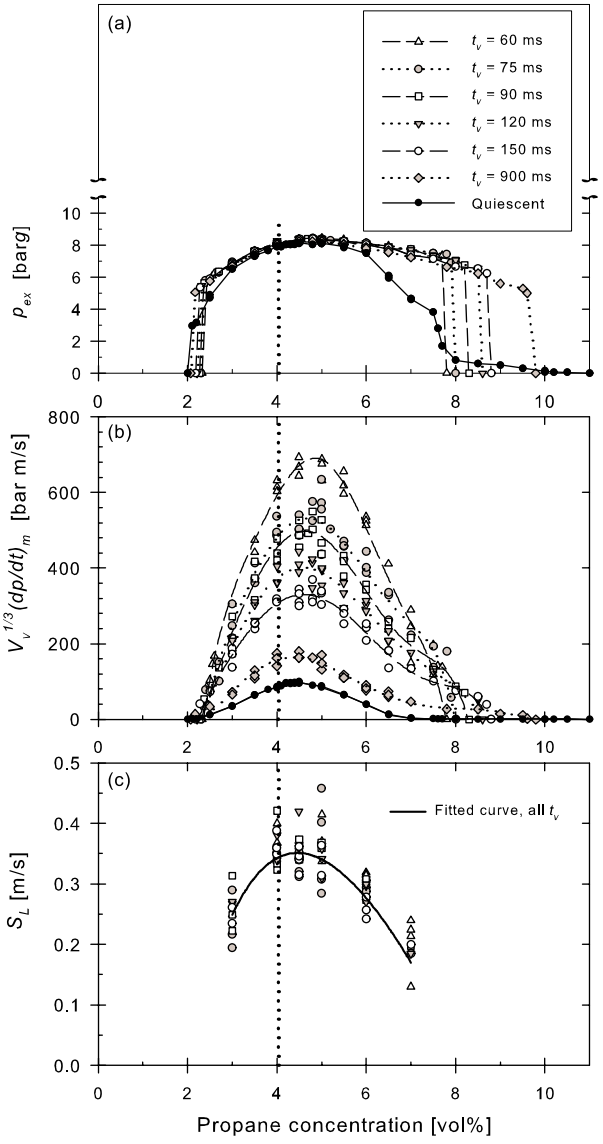

Fig. 1. Flammability data for propane-air mixtures determined in a 20-litre vessel (Skjold, 2003). Laminar burning velocities are estimated for all tests where Eq. (5) is valid (60 ms $< t_{ip} <$ 200 ms). Stoichiometric concentration is indicated by the vertical dotted lines.

Experimental results and estimated laminar burning velocities for maize starch are shown in Fig. 4. In comparison to the results for propane-air mixtures, the corresponding

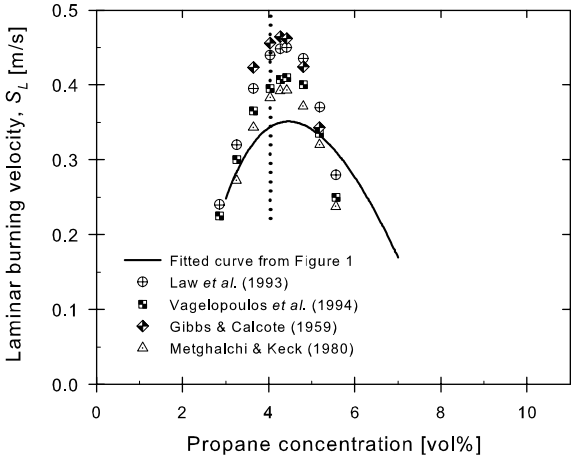

Fig. 2. Comparison between literature data and the estimated laminar burning velocities for propane-air mixtures in Fig. 1.

results for maize starch, at a nominal dust concentration of 800 g m^{-3}, indicate a systematic decrease in estimated laminar burning velocities for longer ignition delay times. This may indicate that the correlations between turbulent and laminar burning velocities for dust clouds deviates from the ones used for gaseous fuels. However, turbulence modulation due to the presence of dust particles, or a systematic difference between real and nominal dust concentrations, may be partly responsible for this result. Due to the large scatter in the results for high dust loading, data for concentrations above 1500 g m^{-3} were not used in the final model.

3.5. Empirical model for maize starch

Because the laminar burning velocities estimated for propane-air mixtures were somewhat lower than values found in literature, the laminar burning velocities for maize starch used as input to DESC was multiplied by a factor of 1.1 in this work. The resulting empirical model is illustrated in Fig. 5; it includes the estimated laminar burning velocities

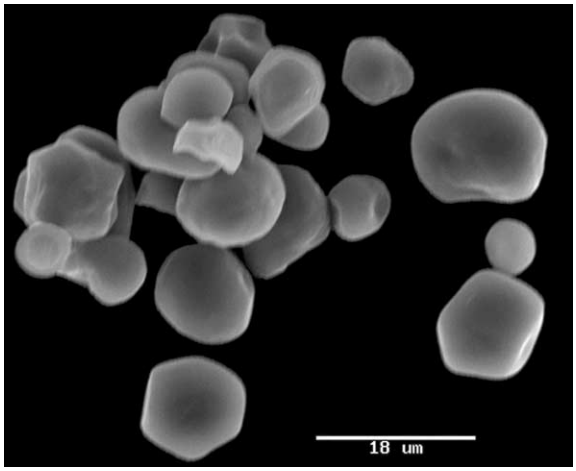

Fig. 3. SEM picture of maize starch particles (Meritena A).

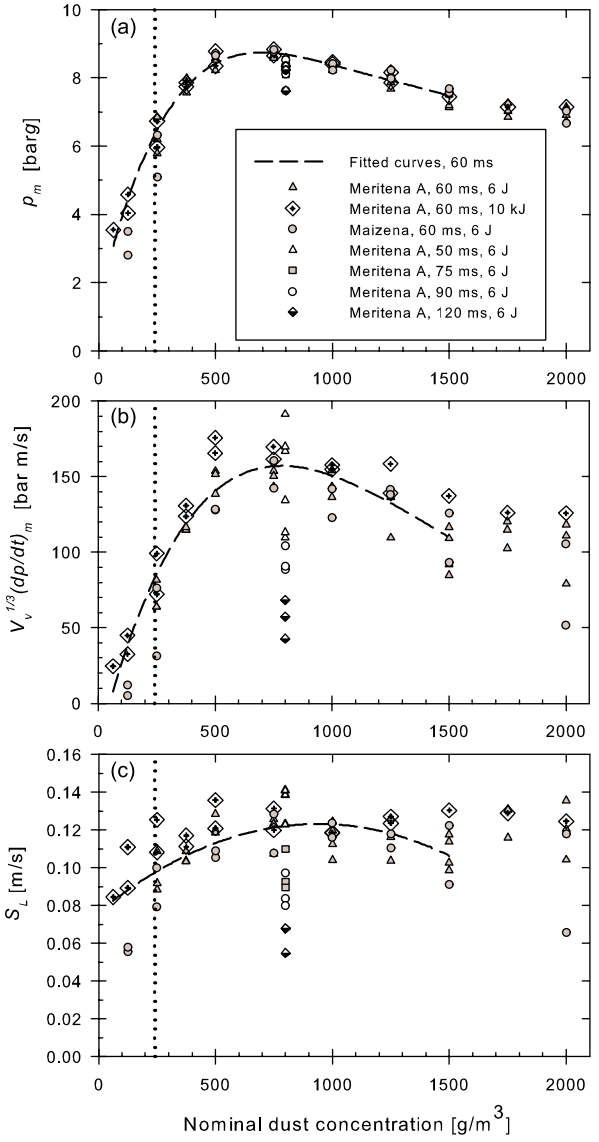

Fig. 4. Experimental results for maize starch: corrected explosion pressures (a), size corrected rates of pressure rise (b), and estimated laminar burning velocities (c). Fitted lines represents values used as input to the model in DESC. Stoichiometric concentration is indicated by the vertical dotted lines.

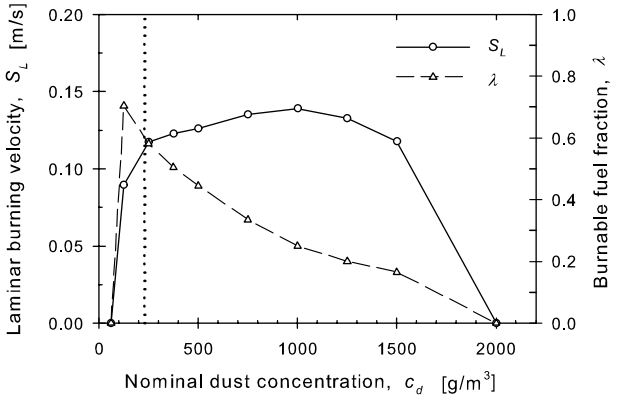

Fig. 5. Empirical input to DESC for maize starch.

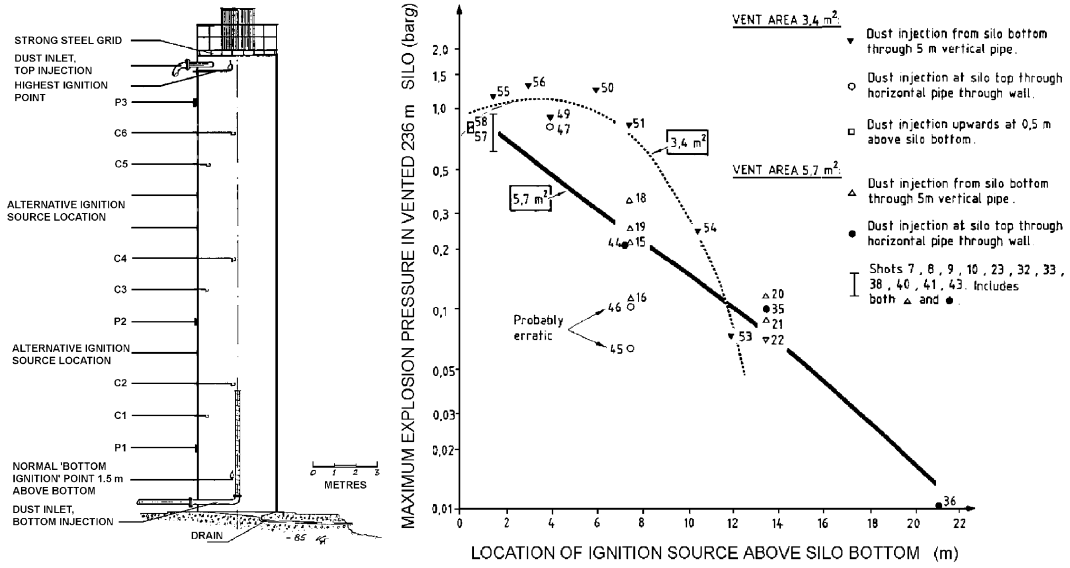

Fig. 6. Vertical section of experimental silo (left), illustrating injection points, ignition positions, pressure probes (P1–P3) and dust concentration probes (C1–C6), and summary of experimental results (right); both from Eckhoff et al. (1985).

and the estimated fraction of fuel that is allowed to react, as a function of dust concentration (c_d). Lower and upper flammability limits are estimated to 60 and 2000 g m^{-3}, respectively.

4. Simulation of vented maize starch explosions

In this section, the empirical model illustrated in Fig. 5 is used to simulate a series of large-scale maize starch explosion experiments in a vented 236-m^3 silo (Eckhoff et al., 1985, 1987).

4.1. Experiments and experimental results

A vertical cross-section of the silo is illustrated in Fig. 6; the silo was 22 m high and 3.7 m in diameter. Two different vent areas were used: 3.4 and 5.7 m^2. Explosive clouds of maize starch were generated in three different ways by conventional pneumatic injection:

- Dust injection upwards from the silo bottom through a 5 m vertical pipe with inner diameter 155 mm and pipe exit about 5.5 m above silo bottom. Typical injection time in the experiments were 14 s with an average dust concentration in the pipe of 13 kg m^{-3} and airflow about 2200 m^3 h^{-1} standard state.
- Dust injection upwards from the bottom of the silo bottom without the 5 m pipe (not simulated in this work).
- Dust injection at the silo top through a horizontal pipe. Typical injection time was 22 s with an average dust concentration in the pipe of 9–10 kg m^{-3}.

The dispersed clouds were ignited at various levels above the bottom of the silo. The ignition source was 50 g of dried nitrocellulose powder (200 kJ) contained in a plastic bag, and fired by a fuse head. The average dust concentration in the silo was estimated by measurements with dust concentration probes and weighing of dust gathered from the bottom of the silo. The experimental results is summarised in Fig. 6, and a picture of a vented explosion is included in Fig. 9. The experiments confirmed that for explosions in large elongated silos, vented at the top, the maximum explosion pressure depends strongly on the vertical distance between the vent and the ignition point. Ignition close to the silo bottom generated overpressures exceeding one bar, whereas ignition close to the vent at the top of the silo gave only marginal overpressures, about 10–20 mbar.

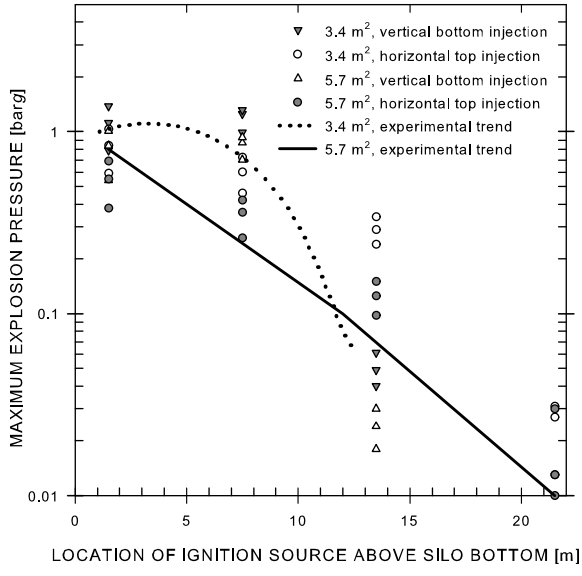

Fig. 7. Influence of ignition position, vent area and dust injection method on maximum simulated explosion pressure; the experimental trend lines from Fig. 6 are indicated for comparison.

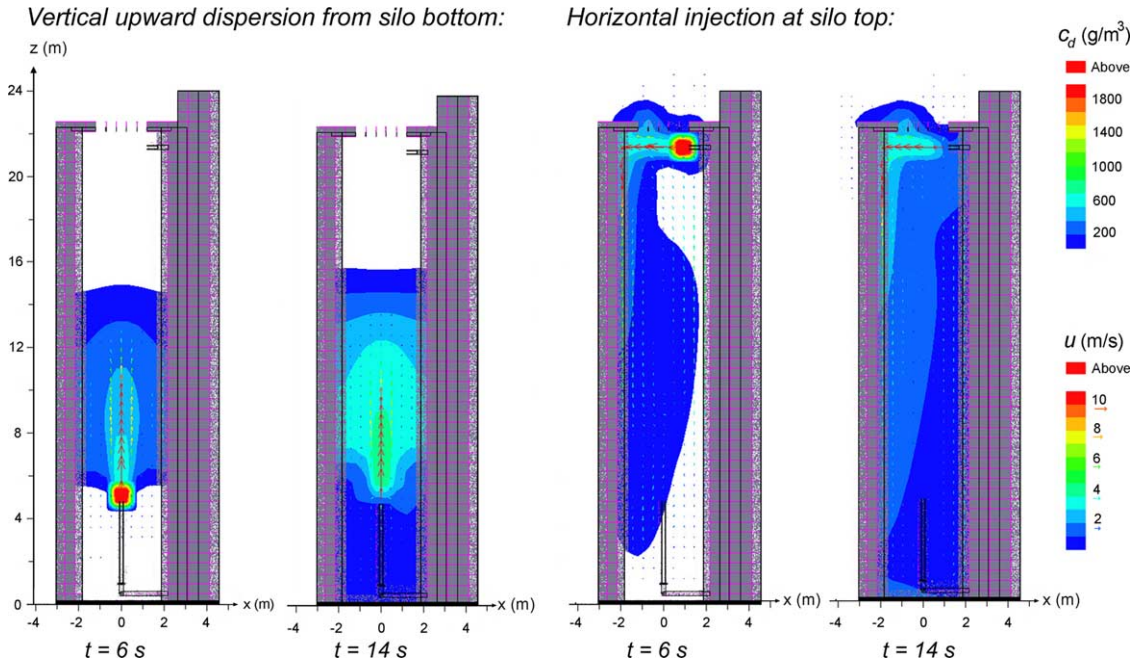

Fig. 8. Simulated dust concentrations and velocity vectors for both vertical upward injection from the bottom of the silo, and horizontal injection at the silo top; two time steps are shown for each scenario. Dust concentrations below 60 g m^{-3} are not shown.

4.2. Simulations and simulated results

From the experiments described by Eckhoff et al., a set of representative explosion scenarios was simulated with DESC. Since much work remains on both modelling and validation of the DESC code, only a qualitative comparison between experimental and modelled results will be attempted here. The total amount of injected dust was reduced to 75 kg in all

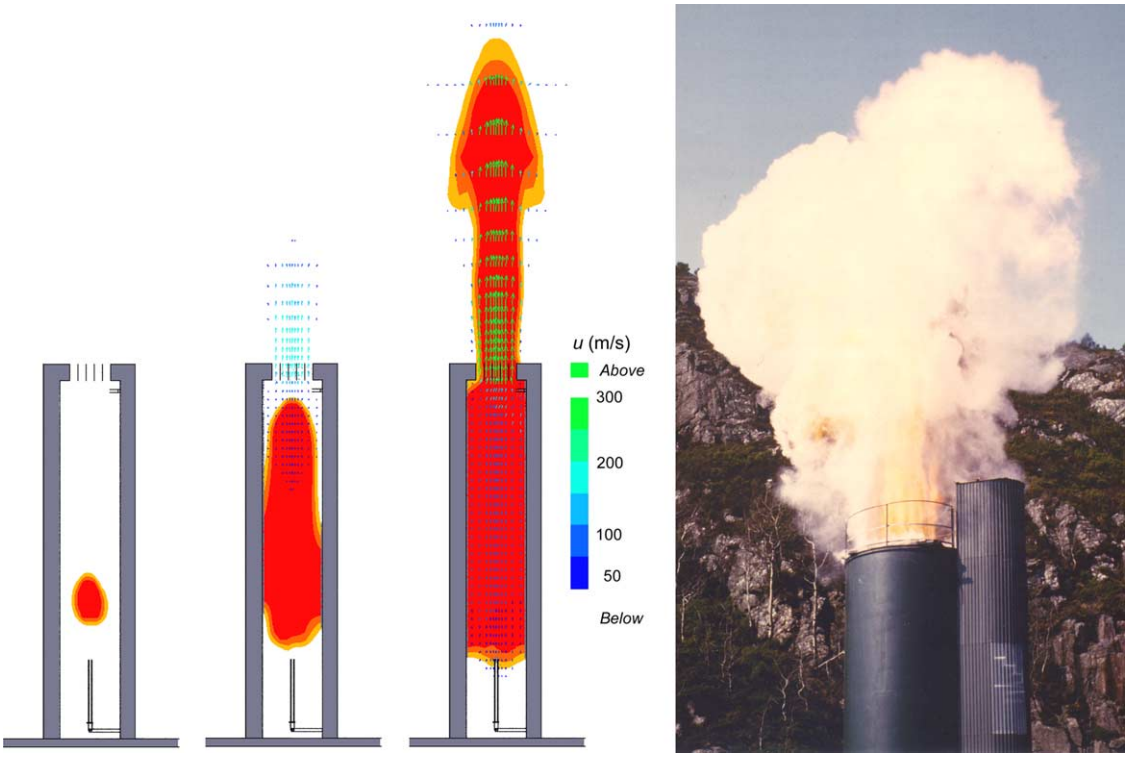

Fig. 9. Simulated velocity vectors and flame development (represented by combustion products) at three selected time steps during an explosion simulation (left); vented dust flame and cloud of maize starch from the actual experiments (right).

simulations, compared to typically 100 kg for bottom injection, and 150 kg for top injection, in the experiments. This reduction seemed reasonable since the resulting average dust concentration of about 320 g m^{-3} is still higher than most of the reported average concentrations from the experiments. The injection process lasted for 14 s in all dispersion simulations; longer dispersion times in experiments with injection at the silo top were needed due to experimental difficulties emptying the horizontal pipe. Four ignition positions were investigated: 1.5, 7.5, 13.5 and 21.5 m above silo bottom. For each ignition position, three explosion simulations were started from the initial conditions defined by the dispersion simulations: −2.4, 0.1 and 2.6 s relative to termination of dust injection. Simulated results are summarized in Fig. 7, and plots illustrating dust injection, flame propagation and pressure development are shown in Figs. 8 and 9. No comparison between measured and simulated flame propagation has been attempted at this stage, and it should be noted that a relatively coarse grid, 0.5-meter cubical grid cells, has been used in the simulations.

5. Discussion

Although there is significant scatter in both experimental and simulated results, the simulated explosion pressures in Fig. 7 agree reasonably well with the experimental results in Fig. 6. The highest overpressures in both simulations (1.3–1.4 bar) and experiments (1.2 bar) were found for the smallest vent area (3.4 m^2), with dust injection from the bottom of the silo, and ignition in the lower part of the silo. A high vented explosion pressure seems to be favoured by higher initial burning rates for early ignition due to higher pre-ignition turbulence generated by dust injection, and longer vertical distances from the ignition point to the vent, resulting in turbulence enhancement by expansion-generated flow. Fig. 8 illustrates that with injection from the bottom, concentrations in the simulated dust cloud are below the lower flammability limit in the upper part of the silo. Hence, there are no simulated explosion pressures for bottom injection and ignition 21.5 meters above the silo bottom. However, lower simulated explosion pressures (20–30 and 40–60 mbar for 5.7 and 3.4 m^2 vent areas, respectively) with bottom injection and ignition at 13.5 m, compared to the experimental values close to 0.1 bar, indicates that simulated dust concentrations in the upper part of the silo may be too low. Simulation of dispersion processes should become more realistic if improved modelling of two-phase flow can be included in later versions of DESC.

The simple method of generating an empirical model from experimental data obtained in a 20-litre explosion vessel seems to work reasonably well for this particular case. However, much work remains on both modelling and validation. There are several uncertainties associated with the chosen approach, such as:

- It is not straightforward to determine the laminar burning velocity for dust clouds (Dahoe et al., 2002; Krause & Kasch, 2000; Lee, 1988), and this makes it difficult to validate the laminar burning velocities estimated by the method used this work.
- Combustion of dust-air clouds is characterized by a higher degree of volumetric energy release, compared to premixed gaseous flames (Lee, Pu, & Knystautas, 1987); hence, flame thickness can be expected to have strong influence of on pressure-time curves from dust explosions in closed vessels (Dahoe et al., 1996).
- The results are sensitive to uncertainties in the estimates of ℓ_m and u'_{rms} during the decay of turbulence in the 20-litre vessel.
- The applicability and accuracy of the correlations used to estimate the turbulent burning velocity remains to be verified.

Further details are discussed by Skjold et al. (2005).

6. Conclusions

Experimental results for maize starch obtained in a 20-litre explosion vessel have been used as input for the combustion model in an early version of the CFD-code DESC. Simulation of various dust explosion scenarios in a vented 236-m^3 silo reproduces trends found in the experiments reasonably well. Although much work remains on both modelling and validation, increased understanding of the dust explosion phenomenon will be gained through the development of CFD-codes for dust explosion modelling.

Acknowledgements

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