POSSIBILITIES, LIMITATIONS, AND THE WAY AHEAD FOR DUST EXPLOSION MODELLING

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The purpose of the present paper is threefold. First, a brief review of modelling, main results, and preliminary conclusions from the DESC project are presented; current capabilities and limitations of the DESC code are discussed. Second, it will be demonstrated how a CFD-code for dust explosions can be used as a valuable tool by industry, consultants, researchers or regulatory authorities in order to fulfil more effectively the requirements of the ATEX directives. Third, some thoughts on the way ahead for dust explosion modelling are outlined in the light of both current knowledge about dust explosions, and inherent limitations in modelling capabilities of present CFD-codes.

INTRODUCTION

A dust explosion can be defined as the rapid combustion of a cloud of combustible dust. Since the fuel can be any finely divided solid material, typically 1–100 μm in diameter, capable of reacting rapidly and exothermically with a gaseous oxidizer, dust explosions represent a hazard to both personnel and equipment in industries that handle combustible powders. Accidental dust explosions always involve turbulent flow: turbulence is required for generating the explosive dust cloud, and additional turbulence is produced during the explosion. Hence, any model aimed at realistically describing the dust explosion phenomenon should include the effect of turbulence on flame propagation. Since physical initial and boundary conditions also have strong influence on the course of explosions, the model should also allow for a reasonably accurate description of the actual geometry. Other parameters that should be taken into account include the initial flow field, the chemical composition of the dust, the particle size distribution, the dust concentration, the location of the ignition source and the possibility of entraining additional dust from dust deposits.

Computational fluid dynamics (CFD) is a science that utilizes numerical methods and digital computers to produce quantitative predictions of fluid-flow phenomena based on conservation equations for mass, momentum, and energy. Provided appropriate models for particle-laden flow and turbulent heterogeneous combustion can be identified and implemented, CFD codes for dust explosions may become valuable tools for the design of process plants and explosion mitigation systems. The main aim of the DESC project has been to develop a simulation tool based on CFD that can estimate the course of industrial dust explosions in complex geometries.

The reactivity of explosive dust clouds is often characterized by the K_{St} value, defined as the maximum rate of pressure rise, multiplied by the cube root of the vessel volume. The limitations of the 'cube-root-law' when it comes to scaling dust explosions are well known (Eckhoff, 1984; Dahoe, 2001ab). Nevertheless, since practically all standardized methods for determining the reactivity of dust clouds are based on tests performed in closed explosion chambers, either 1-m^3 or 20-litre or in volume (ISO, 1985; Cesana and Siwek, 2001), it is tempting to explore the possibility of utilizing the data obtained in such tests as input to combustion model for dust clouds. This approach has been adopted for the first version of the new CFD-code DESC (Dust Explosion Simulation Code).

DESC – DUST EXPLOSION SIMULATION CODE

THE DESC PROJECT

The DESC project was initiated early 2002 and ended in 2004. The European Commission supported the project through Fifth Framework Programme called Competitive and Sustainable Growth (GROWTH). The project included extensive experimental work, measurements in real process plants, modelling and validation. The DESC consortium had the following participants: Health and Safety Laboratory (HSL), GexCon, Nederlandse Organisatie voor Toegepast-Natuurwetenschappelijk Onderzoek (TNO), Fraunhofer ICT, Inburex GmbH, Warsaw University of Technology, Delft University of Technology, Forschungsgesellschaft für angewandte Systemsicherheit und Arbeitsmedizin (FSA), Øresund Safety Advisers AB, Hahn & Co, and Lyckeby Culinar AB; contributions were also received from Fike Europe, INERIS, and University of Bergen.

THE DESC CODE

DESC is based on the existing CFD code FLACS for gas explosion modelling. The first version of the DESC code was release in October 2005, and although some of the work on validating the code has been delayed, promising results have already been obtained for fine organic dusts (Skjold et al., 2005ab). The mitigating effect of vent panels and fast acting valves can be modelled, and work is on the way to include the effect of suppression systems. However, the current version of DESC cannot model detonations and explosions involving metals or hybrid mixtures. Particle-laden flow is modelled by the Eulerian approach in the limiting case when the Stokes number approaches zero, so-called equilibrium mixtures (Crowe et al., 1998). It is assumed that the dispersed dust particles are in dynamic and thermal equilibrium with the gaseous phase. The main reason for not utilizing more advanced models for particle-laden flow is limitations in the currently used combustion model.

In order to overcome some of the difficulties associated with the unambiguous determination of fundamental flame propagation properties for dust clouds, the approach adopted for the first versions of DESC has been to estimate such parameters from pressure-time histories measured in standardized 20-litre explosion vessels (Figure 1).

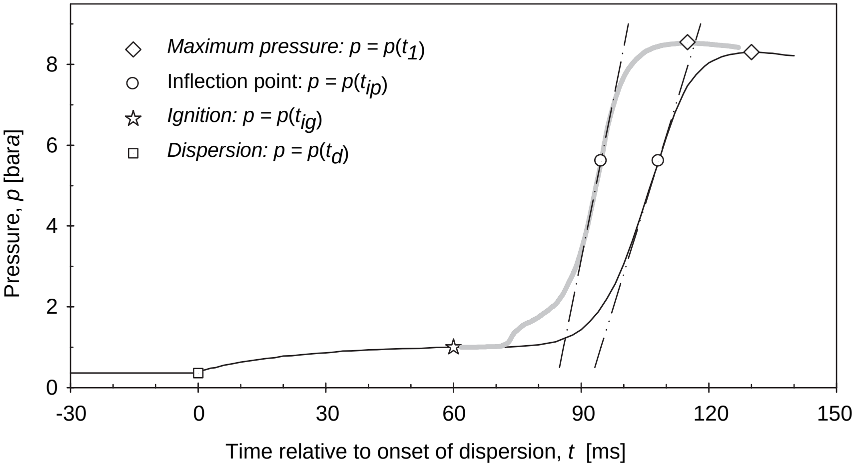

Figure 1. Typical pressure-time curves obtained from dust explosion tests in 20-litre explosion vessels; the thin black curve is obtained in a test ignited with a 6 J electric arc, and the thick grey curve illustrates the influence of two 5 kJ chemical igniters on the pressure development

The procedure followed in order to generate empirical input to the combustion model in DESC from pressure-time curves is outlined in the following. Turbulent burning velocities are extracted from experimental pressure-time curves by a method suggested by Pu *et al.* (1990); the following equation, derived from a two-zone model (Dahoe, 1996), is currently used:

$$S_T(t_{ip}) = \frac{1}{3[\hat{p}(t_1) - p(t_{ig})]}\left(\frac{dP}{dt}\right)_m \left(\frac{3V_v}{4\pi}\right)^{1/3}\left(\frac{p(t_{ip})}{p(t_{ig})}\right)^{-1/\gamma} \left\{1 - \left(\frac{\hat{p}(t_1) - p(t_{ip})}{\hat{p}(t_1) - p(t_{ig})}\right)\left(\frac{p(t_{ip})}{p(t_{ig})}\right)^{-1/\gamma}\right\}^{-2/3} \tag{1}$$

where V_v denotes the volume of the explosion vessel; $(dp/dt)_m$ is the maximum rate of pressure rise (measured in the inflection point); t_{ig}, t_{ip} and t_1 define the time of ignition, maximum rate of pressure rise and maximum pressure, respectively (Figure 1); $\hat{p}(t_1)$ is the maximum absolute explosion pressure corrected for the effect of the ignition source and heat loss to the vessel walls (usually reported as the corrected maximum overpressure p_m). In the future, equation (1) should probably be replaced with a more advanced three-zone model in order to better account for the thickness of the flame (Dahoe, 1996). The root-mean-square of the turbulent velocity fluctuations (u'_{rms}) in the inflection point is estimated from a decay law for the transient flow in a 20-litre sphere equipped with a rebound nozzle (Dahoe, 2000):

$$\frac{u'_{rms}(t_{ip})}{u'_{rms}(t_0)} = \left(\frac{t_{ip}}{t_0}\right)^{-n} \qquad 0.060\,s < t_{ip} < 0.200\,s \tag{2}$$

with the constants $u'_{rms}(t_0) = 3.75$ m s^{-1}, $t_0 = 0.060$ s and $n = 1.61$ (Figure 2). An integral turbulent length scale is estimated by a slightly modified version of an empirical decay formula presented by Dahoe (2000):

$$\ell_I(t_{ip}) = \min\begin{cases} \ell_I(t_0) \cdot \exp\left(a_1 \ln\left(\frac{t}{t_0}\right) + a_2\left\{\ln\left(\frac{t}{t_0}\right)\right\}^2\right) \\ \ell_{I,\ \max} \end{cases} \tag{3}$$

$$\times\, 0.070m < t_{ip} < 0.200s$$

where $\ell_I(t_0)$ is about 0.013 m, t_0 is 0.0588 s, a_1 and a_2 are -3.542 and 1.132, respectively, and $\ell_{I\max}$ is 0.004 m (Figure 2).

Following an approach suggested by (Bradley *et al.* 1988), the default correlation for the turbulent burning velocity in DESC is the following version of the general expression presented by Bray (1990) for gaseous fuels:

$$S_T = 15.1 \cdot S_L^{0.784} \cdot u'^{0.412}_{rms} \cdot \ell_I^{0.196} \tag{4}$$

Other tools for simulating the consequences of dust explosions are using the same type of correlations (Proust, 2005). Laminar burning velocities are estimated from pressure time

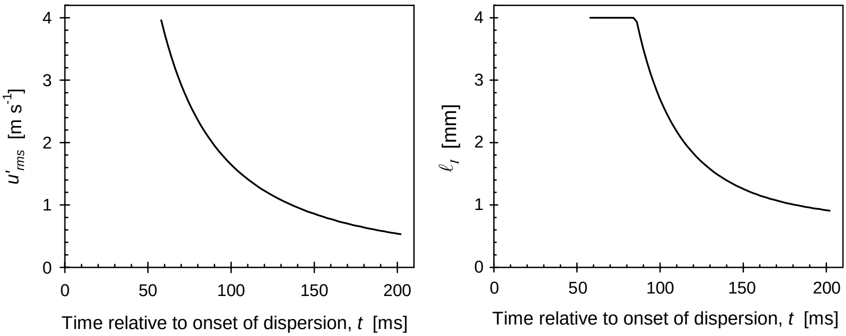

Figure 2. The empirical decay laws for the root-mean-square of turbulent velocity fluctuations (left) and turbulent integral length scale (right) in standardized 20-litre explosion vessels

curves measured in standardized 20-litre vessels with an inverse version of equation (4), using the estimated values obtained from equations (1), (2) and (3):

$$S_L(t_{ip}) = 0.0313 \cdot [S_T(t_{ip})]^{1.276} \cdot [u'_{rms}(t_{ip})]^{0.526} \cdot [\ell_I(t_{ip})]^{-0.25} \tag{5}$$

The mass fraction of fuel that is converted to products, λ, is defined as the amount of fuel that must react in order to produce the corrected explosion pressure, p_m, taking into account both the heats of formation, and the ratio between gaseous species, in reactants and products. Estimated values for S_L and λ are used as empirical input to the combustion model in DESC.

During an explosion simulation, turbulent burning velocities are found from equation (4); $u'_{\max}$ is taken from the traditional two-equation k-ε model (Lauder and Spalding, 1974), and the integral length scale ℓ_I is estimated from the following equation:

$$\tilde{\ell}_I = \min\begin{cases} 0.025 \cdot r_F \\ 0.08 \cdot L_S \end{cases} \tag{6}$$

where r_F is the flame radius and L_S is the minimum spatial dimension of enclosures constraining the flame (e.g. the smallest dimension of a duct the flame propagates through). Length scales derived from the k-ε model are not currently used in the combustion model because such estimates depend strongly on the resolution of the computational grid.

APPLICATIONS

According to new European legislation, it is now compulsory for employers to evaluate the risk posed by dust explosions in their facilities, and to document that adequate safety measures have been taken (ATEX 1999/92/EC); it must also be documented that equipment intended for use in potentially explosive atmospheres are safe to operate (ATEX 94/9/EC). In order to estimate the risk, one must assess both the probability for various explosion scenarios to occur, and the consequences of such events. Since the determination of both flame propagation and pressure build-up are of vital importance when estimating the consequence of explosions, results from CFD simulations are relevant during the design of powder handling plants, when optimising mitigating measures, and during forensic investigations of accidents that have taken place. Typical calculations that might be of interest include:

- Optimising the design of mitigating measures, including finding suitable locations for pressure and flame detectors, vent panels, rupture discs, vent ducts, suppression canisters, fast acting valves, etc.
- Estimating pressure loads due to blast waves from vented explosions on buildings and other structures
- Extrapolating experimental test data during certification processes for equipment intended for use in explosive atmospheres

- Identifying hazardous areas in process plants
- Investigating the probability and consequences of escalating explosion scenarios

CFD codes are particularly well suited for investigating explosion scenarios in complex geometries such as venting of elongated vessels and interconnected vessel systems. The next section presents an example where DESC is used as a supplement to existing standards and guidelines during the evaluation of mitigating measures in a process plant.

VENTING A DRYER THROUGH A DUCT

This section illustrates how DESC was used to investigate explosion protection of a so-called multicoil dryer. In one end of the dryer, wet product is injected with a conveyor worm. The product is then transported towards the other end of the dryer by a rotating multicoil system, constantly being stirred and heated. Dried product particles are entrained by the flow of hot air and exit through an outlet pipe. The material in question was a copolymer, typical particle size 10–15 μm.

The total volume of the dryer is about 13-m^3, and although it has been designed to withstand a maximum overpressure $p_{red,max}$ of only 0.3 bar*g*, the construction may readily be reinforced to withstand 0.5 bar*g*. The existing explosion mitigation consists of two vent panels, leading into an 8 m long vent duct with a 90° bend. The total vent area for both panels is 1.0-m^2, opening pressure p_{stat} 0.1 bar*g*. According to the European standard on dust explosion venting (prEN14491, 2004), the minimum vent areas without any duct should be 2.0 and 1.3 m^2 for $p_{red,max}$ equal to 0.3 and 0.5 bar, respectively. Although the standard does not contain any methodology for the design of vent ducts with 90° bends, a reference is made to the guidelines from IChemE (Barton, 2002). Since the existing explosion mitigation of the dryer seems inadequate according to current standards, a new vent duct design has also been considered; with the modified design the total vent area can be doubled. Installation of a suppression system has been considered, but the risk of ruining entire batches of product by accidentally releasing suppressant into the dryer, combined with the additional cost of installation and maintenance, has so far rendered passive mitigation systems more attractive.

In order to generate an empirical model for DESC, samples of both wet and dried material were tested in 20 litre explosion vessels; the results are summarized in Figure 3. Tests with arc ignition were performed in a modified 20-litre USBM vessel at the University of Bergen, and tests with chemical igniters were performed in a standardized 20-litre Siwek-sphere at GexCon AS; test procedures are described by Skjold (2003) and Cesana & Siwek (2001), respectively. Wet material was difficult to disperse, and could only be ignited with two 5 kJ chemical igniters; the K_{St} value was found to be 17 bar m s^{-1}. The dried product, on the other hand, was easy to disperse, could readily be ignited with the electric arc, and had a K_{St}-value of 240–270 bar m s^{-1}. Hence, a dramatic change in the reactivity of the product takes place when the material is dried. The minimum explosive dust concentration was determined to be 30 g m^{-3}, and it was assumed that the maximum explosive dust concentration is 2500 g m^{-3}. Figure 3 also show the estimated turbulent and laminar burning velocities, following the stepwise procedure outlined above, and the

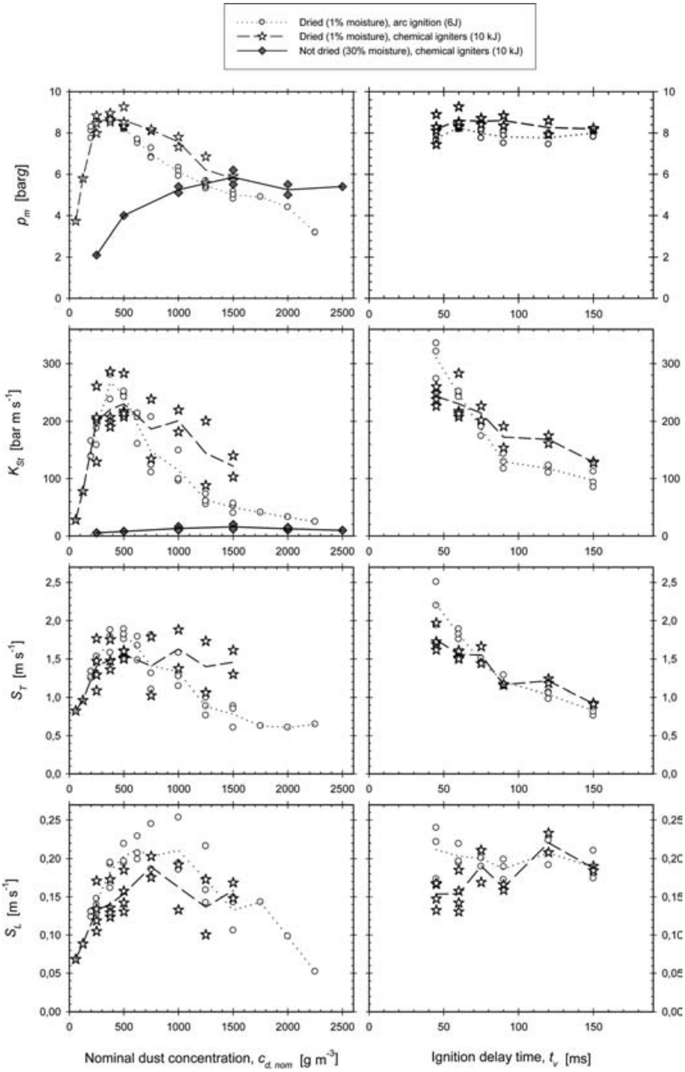

Figure 3. Corrected explosion pressures (p_m), size corrected rates of pressure rise (K_{St}) and estimated laminar and turbulent burning velocities (S_T and S_L) as function of nominal dust concentration (left; $t_v = 60$ ms) and ignition delay time (right; $c_{d,\ nom} = 500$ g m^{-3}) for dried copolymer (1% moisture content); some data are also included for wet material (30% moisture content)

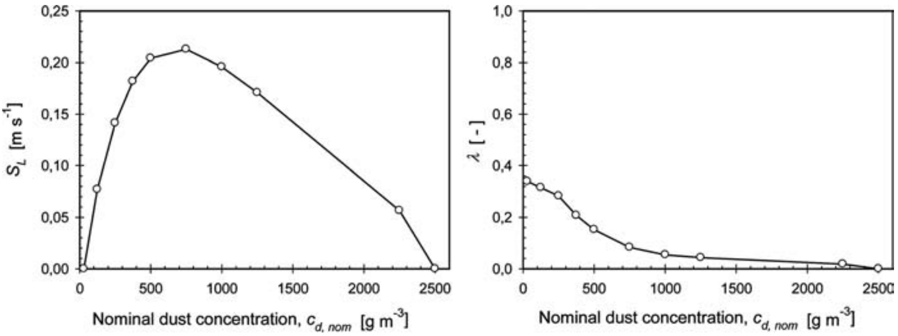

Figure 4. Empirical model in DESC from the data summarized in Figure 3; estimated laminar burning velocity (left) and burnable fraction of fuel (right) as function of nominal dust concentration

effect of varying the ignition delay time (i.e. initial turbulence) in the experiments. The empirical model used by DESC is summarized in Figure 4; it was constructed from the results obtained in the arc ignited tests in Figure 3.

The implemented model for the multicoil dryer with the existing vent duct is illustrated in Figure 5. Worst-case conditions have been assumed to result from a turbulent cloud with dust concentration 400 g m^{-3} filling the entire dryer. Since it seems highly unlikely that such a worst-case dust cloud can be generated inside the entire drier, a reduced dust cloud, occupying only about one third of the total volume, has also been

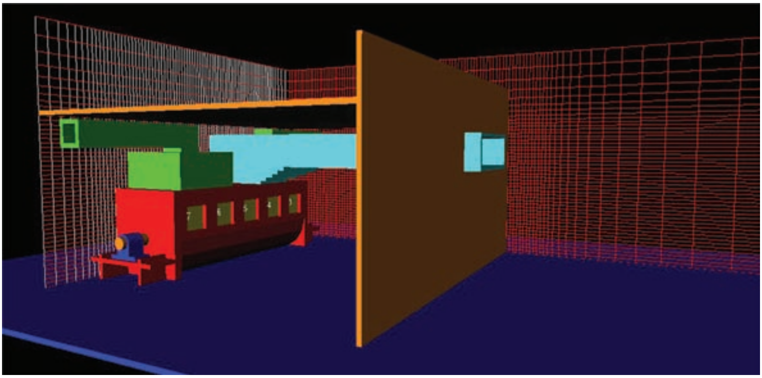

Figure 5. Implemented geometry of multicoil drier, illustrating the computational grid; 0.1 m cubical grid cells are used throughout the interior of both the dryer and the vent duct, and the grid cells are stretched outside this region

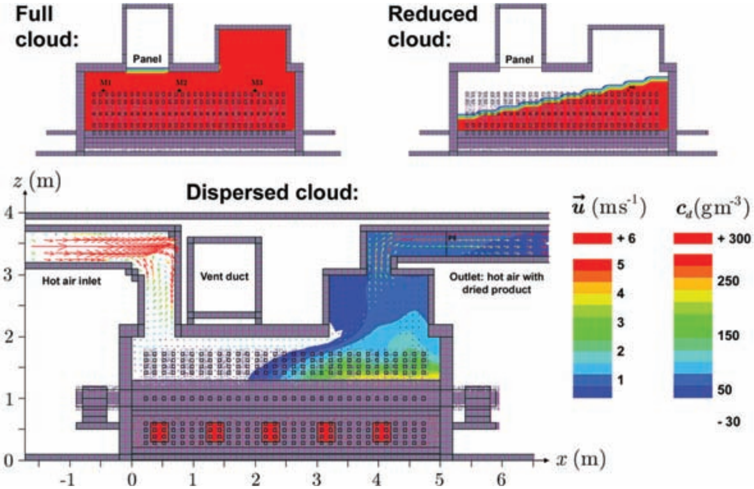

Figure 6. Vertical cross sections of multicoil drier, illustrating the various initial dust clouds used in the explosion simulations: *worst-case cloud* (400 g m^{-3} in the entire dryer), *reduced cloud* (about one third of the dryer volume filled with cloud, 400 g m^{-3} in), and *dispersed cloud* (resulting from simulating the flow of air through the dryer while injecting dust from the bottom). The lower plot is a cross-section along the centre of the dryer (through the shaft, $y = 0$), while the cross sections in the upper plots are at $y = 0.3$ meters

investigated. In order to imitate dust clouds generated during normal production, the normal flow of air through the drier was simulated while dust was injected from a porous layer in the bottom at rate corresponding to the maximum production rate. The explosive part of the resulting dust cloud occupied only about half the dryer volume (average concentration 100 g m^{-3}). The three dust clouds that were used as initial conditions for the explosion simulations are illustrated in Figure 6. Since flameless venting also has been considered, the effect of additional venting directly from the dryer was simulated by allowing two or four of the five doors, shown in Figure 6, to function as an additional vent panel; each door represented a vent area of 0.36 m^2. Two quite hypothetical scenarios were also investigated: no multicoil system inside the dryer (less turbulence generation), and venting without the vent duct (to illustrate the effect of the duct). For each scenario, three different ignition positions were used.

The pressure-time curves for the various explosion scenarios are summarized in Figure 7, and some vented explosions are illustrated in Figure 8. The following observations may be noted, assuming the simulation results are reliable:

- If dust explosions are initiated in a worst-case dust cloud, and vented through the existing duct, the pressures can reach 2–3 bar*g*; by either going to a reduced dust cloud,

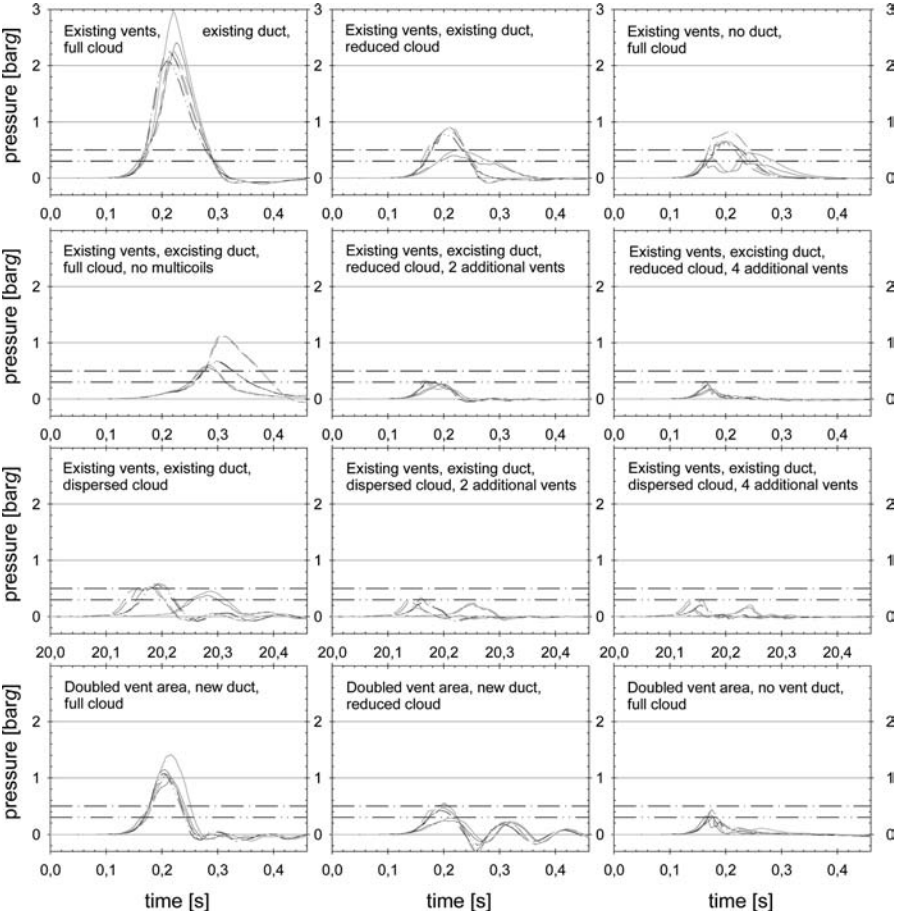

Figure 7. Simulated explosion pressures as function of time for various combinations of initial dust clouds, vent areas and vent duct designs; each plot contain results from three different ignition positions, and pressures in two positions, *M1* and *M3* in Figure 6, are plotted for all simulations. Horizontal lines at 0.3 (and 0.5) bar*g* indicate the design pressure of the dryer (and reinforced dryer)

or removing the vent duct, the pressure is reduced to 0.5–0.8 bar*g*; with no multicoil system, the pressure is reduced to 0.6–1.1 bar*g*, and the pressure peak is delayed by about 0.1 s (this illustrates the effect of internal on turbulence production during the explosion).

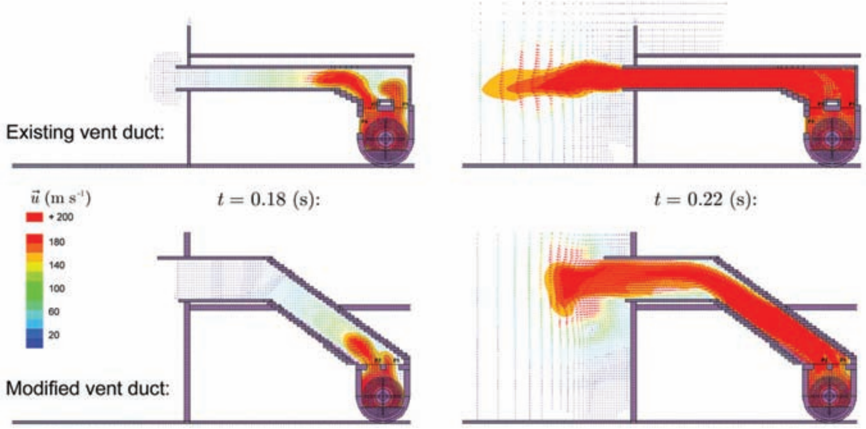

Figure 8. Cross-sections showing velocity vectors and flame propagation for explosion simulations in the existing duct (above) and the modified duct (below) at two selected time steps

- If dust explosions are initiated in the dispersed dust cloud, and vented through the existing duct, the maximum pressures are in the range 0.3–0.5 bar*g*; with moderate additional venting directly from the dryer the pressures are decreased to less than 0.3 bar*g* for both the reduced and dispersed cloud.
- The modified vent duct design results in pressures in the range 1.0–1.4 bar*g* for the full cloud and 0.3–0.5 bar*g* for the reduced cloud; with no duct, the pressure is 0.3–0.34 bar*g* which is consistent with current guidelines for venting (prEN14491, 2004).

It is not straightforward to draw any unambiguous conclusions based on the results presented above; there are uncertainties associated with both the results from the simulations, and the choice of initial conditions. It nevertheless seems likely that the dryer would be reasonably well protected if the new duct and doubled vent area were combined with reinforcing the dryer; a few additional flames venting devices positioned near the outlet should also be considered in order to obtain more distributed venting of the enclosure.

FUTURE PROSPECTS FOR DUST EXPLOSION MODELLING

The new ATEX directives seem to open up for a more differentiated approach to design of explosion mitigation systems in Europe. Given the nature of the dust explosion phenomenon, especially the strong influence of initial and boundary conditions on the course of industrial dust explosions, it seems inevitable that computational fluid dynamics will play an increasingly important role both during the design of new process plants,

Table 1. Summary of some of the physical and chemical processes and properties that may be relevant with regards to dust explosion modelling

Flow related processes	Combustion related processes	Fuel related properties
Agglomeration	Chemical kinetics	Chemical composition
Dust lifting	Devolatilisation	Volatile content
Dust settling	Pyrolysis	Moisture content
Particle-laden flow	Heterogeneous combustion	Particle size distribution
Transient flow	Flame acceleration	Heat of formation
Turbulent flow	Turbulent combustion	Specific heat capacity
Single particle movement	Single particle combustion	Thermal conductivity

and when installing systems for explosion mitigation. However, it is a challenge to model transient turbulent reacting multiphase flow through complicated geometries, and the complexity of the problem necessitates a number of simplifications. The success or failure of a CFD-code when it comes to predicting the course of realistic industrial dust explosions will depend on the modeller's ability to identify and handle the most significant physical and chemical processes that are involved in dust explosions (Table 1 and Figure 9).

There are many pitfalls associated with the pragmatic modelling approach adopted for the first version of DESC. There are significant uncertainties associated with both the

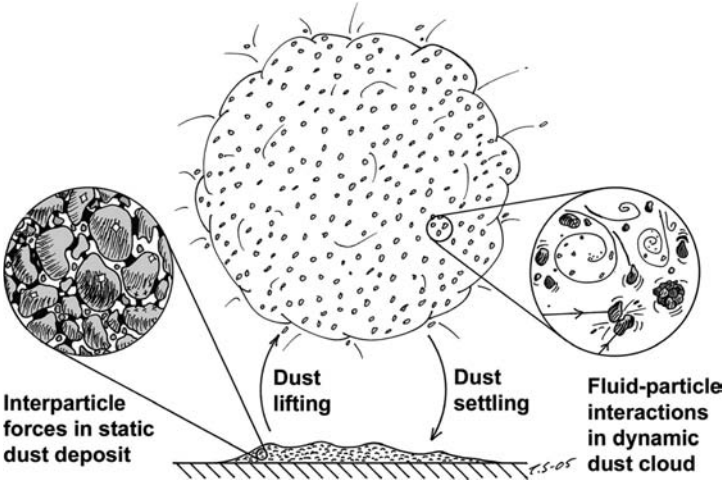

Figure 9. Phenomena that should be modelled in order to describe the generation of combustible dust clouds

simplified modelling of particle-laden flow, and the use of correlations such as equation (4) to describe turbulent dust flames (Skjold *et al.*, 2005d). Although the method used for extracting laminar burning velocities from pressure-time curves obtained in 20-litre vessels seems to work reasonably well for turbulent propane-air mixtures (Skjold *et al.*, 2005c), the use of this method may be more questionable when it comes to dust flames (due to the thickness of the flame). It may also be somewhat problematic that the generation of an empirical model, such as the one illustrated in Figure 4, requires data from experiments (Lee, 1988). It is sometimes argued that one should be able to calculate fundamental combustion properties, such as the laminar burning velocity, from first principles; however, one should keep in mind that such an approach is hardly possible to carry out even for gaseous fuels. Most CFD-codes that are used to simulate large scale industrial gas explosions utilize experimentally determined laminar burning velocities as input. Factors such as the solvers and numerical schemes used in the code, the type of computational grid, the turbulence and combustion models, the grid resolution, etc., may also influence the results obtained with a CFD code.

Consequence analysis by CFD in powder handling plants can be done at various levels of sophistication. In certain situations it may be advisable to follow a *worst-case approach*, i.e. searching for the ignition position that causes the most severe consequences, assuming the entire enclosure initially filled with a highly turbulent dust cloud of the most reactive concentration. More often, however, it is practically impossible, or unnecessarily expensive, to design according to the worst-case scenario, and a *realistic worst-case approach* may seem more appropriate. Typical circumstances that usually will result in less devastating consequences include coarser particle size distributions, higher moisture content, enclosures that are only partly filled with explosive dust clouds, dust concentrations that differ significantly from the most reactive concentration, quenching of dust flamed due to high strain rates or heat loss, and lower levels of initial turbulence in the cloud. Design based on *realistic process conditions* has been suggested (Siwek *et al.*, 2004). The main challenge associated with adopting a less conservative approach is to identify all explosion scenarios that are reasonably likely to occur in practice, and not overlooking factors that may cause such event to escalate (e.g. pressure piling and jet ignition in connected vessels, dispersion of dust deposits by flow or shock waves, and transition to detonation). Since accidental dust explosions very often occur during extraordinary conditions, such as start-up or shut-down of process plants (Eckhoff, 2003), realistic process conditions may not always provide a relevant description of the initial conditions. A more comprehensive approach to risk assessment could involve quantitative risk analysis (QRA), assigning probabilities to a set of plausible event, and estimating the consequences of each event by means of CFD. This *probabilistic approach* is currently used with considerable success in the oil and gas industry (NORSOK Z-013, 2001). However, it is not straightforward to adopt methods developed by the offshore oil and gas industry to onshore powder handling plants.

Some researchers seem to be of the opinion that current attempts at introducing CFD in the field of dust explosion safety are premature, arguing that more fundamental problems, such as the determination of laminar burning velocity, or finding detailed mechanisms for single particle combustion, must be resolved first. This view is in line with the long tradition of reductionism within the philosophy of science. However, since experiments aimed at revealing such fundamental properties only can be performed under idealized circumstances, e.g. microgravity conditions, it could be argued that their relevance with regards to actual industrial situations may be limited. Assuming the 'real' laminar burning velocity for the 'perfectly dispersed' homogeneous dust cloud could be determined, one is nevertheless left with the problem of relating this 'artificially' obtained parameter to 'actual' turbulent burning velocities in the far from perfectly dispersed turbulent dust clouds found in industry. Hence, for complex phenomena such as dust explosions, one should not rule out the possibility that a more holistic approach may serve the progress of science, and particularly safety, just as well as traditional reductionism.

CONCLUSIONS

The first version of the DESC code has been released, and although much of the validation work remains to be done, results so far indicate that the implemented combustion model may work reasonably well for fine organic dusts. The primary focus in the near future will be to apply the current code to various dust explosion scenarios investigated experimentally, either as part of the DESC project, or from other sources. This work will presumably reveal some of the limitations in the current approach, and provide guidelines on how the models can be improved. It seems likely that our understanding of dust explosions will benefit from the interaction between computational fluid dynamics and dedicated experiments at various scales. In a longer perspective, more advanced modelling of particle-laden gaseous flow and heterogeneous combustion should be included. The establishment of this unique code as a tool in the field of dust explosion safety will ensure that it will be maintained and developed further.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge all contributions from the other partners in the DESC project, and the financial support from the European Commission.

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