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Review of the DESC project

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Abstract

Dust Explosion Simulation Code (DESC) was a project supported by the European Commission under the Fifth Framework Programme. The main purpose of the project was to develop a simulation tool based on computational fluid dynamics (CFD) that could predict the potential consequences of industrial dust explosions in complex geometries. Partners in the DESC consortium performed experimental work on a wide range of topics related to dust explosions, including dust lifting by flow or shock waves, flame propagation in vertical pipes, dispersion-induced turbulence and flame propagation in closed vessels, dust explosions in closed and vented interconnected vessel systems, and measurements in real process plants. The new CFD code DESC is based on the existing CFD code FLame ACceleration Simulator (FLACS) for gas explosions. The modelling approach adopted in the first version entails the extraction of combustion parameters from pressure–time histories measured in standardized 20-l explosion vessels. The present paper summarizes the main experimental results obtained during the DESC project, with a view to their relevance regarding dust explosion modelling, and describes the modelling of flow and combustion in the first version of the DESC code. Capabilities and limitations of the code are discussed, both in light of its ability to reproduce experimental results, and as a practical tool in the field of dust explosion safety.

Keywords: Dust explosions; CFD; DESC

1. Introduction

Dust explosions pose a constant threat in industries that handle combustible powders, and since it may be difficult to prevent such events from taking place, safe operation often relies on the ability of explosion mitigation systems to limit their potential consequences. Although the use of existing guidelines provides adequate levels of safety in most situations involving isolated process units, optimal implementation of explosion protection measures in more complex systems requires additional information from more advanced models, such as phenomenological software (Proust, 2005) or computational fluid dynamics (CFD) codes (Bielert & Sichel, 1999; Skjold, Larsen, & Hansen, 2006). Many of the correlations found in current standards and guidelines originate from a limited number of experimental tests, and there are often significant uncertainties associated with extrapolating their predictions significantly beyond the range of conditions covered by the original experiments (Lunn, 2005). Quantitative predictions of fluid-flow phenomena obtained by solving conservation equations for mass, momentum, and energy by numerical methods and digital computers have the potential of covering a much broader range of explosion scenarios, compared to simple empirical correlations. This is particularly important for industrial dust explosions, because it can be difficult to prevent such accidents from escalating through flame acceleration by repeated obstacles (e.g. bucket elevators and mine galleries), secondary explosions (e.g. coal dust explosions in mines), pressure piling and jet ignition in connected vessel systems (e.g. dryers, cyclones and filters), or structural collapse of process units and buildings.

Accidental dust explosions involve transient turbulent reacting multiphase flow, often in complex geometries. The rather ambitious goal of the Dust Explosion Simulation Code (DESC) project was to develop a simulation tool

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based on CFD that could predict the course of such incidents. The project started in 2002, and ended in June 2005. The consortium had the following participants: Health and Safety Laboratory (HSL), GexCon, Nederlandse Organisatie voor toegepast-natuurwetenschappelijk onderzoek (TNO), Fraunhofer Institut für Chemische Technologie (Fraunhofer-ICT), Inburex Consulting, Warsaw University of Technology (WUT), Technische Universiteit Delft (TU Delft), Forschungsgesellschaft für angewandte Systemsicherheit und Arbeitsmedizin (FSA), Øresund Safety Advisers, Hahn & Co, and Lyckeby Culinar. Contributions were also received from Institut national de l'environnement industriel et des risques (INERIS), Fike Europe, and University of Bergen (UiB). The European Commission supported the project through a cost-sharing contract under the Fifth Framework Programme (DESC, 2001). The experimental programme in the DESC project covered a broad range of issues, and involved several types of dust, including potato and maize starch, coal, and silicon. The complex nature of the dust explosion phenomenon necessitated a rather pragmatic modelling approach. It was necessary to seek a balance between sufficiently accurate models for the relevant physical phenomena (e.g. particle-laden flow and turbulent heterogeneous combustion), robust and efficient numerical schemes, simplified user input, and emphasis on a conservative approach to risk assessments. Due to the diversity of dusts processed in industry, and the fact that numerous factors associated with the dispersed particles may influence the reactivity of a dust–air mixture, combustion models in DESC rely on empirical input from standardized tests in the 20-l explosion bomb.

This paper provides a brief overview of the experimental results obtained throughout the DESC project, and outlines the modelling of flow and combustion in the first version of the DESC code. Motivating factors for the experimental work and inherent limitations in the modelling approach are emphasized throughout, and future prospects for CFD modelling of industrial dust explosions are discussed.

2. The DESC project

The various tasks in the DESC project were executed in seven work packages (WPs). The following sections summarize the outcome from the various WPs, with ample reference to published work.

2.1. Turbulent flow measurements

The turbulent flow conditions strongly influence the rate of combustion in a dust cloud. Hence, the main purpose of WP-1 was to measure the decay of dispersion-induced turbulence in various explosion vessels, and to extract empirical decay formulas for the root mean square of the turbulent velocity fluctuations u'_{rms} and the integral turbulent length scale ℓ_I. Of primary importance was the decay of turbulence in 20-l vessels fitted with the default dispersion system from Kühner (Cesana & Siwek, 2001), but measurements in larger vessels were also included.

Zevenbergen (2004a) reported laser Doppler anemometry (LDA) measurements in a 20-l spherical vessel at TU Delft. However, since no explicit decay formulas for turbulence were included in the report, further modelling relied on relations reported by Dahoe, Cant, and Scarlett (2001) and Dahoe, van der Nat, Braithwaite, and Scarlett (2001). HSL used an LDA system to measure the decay of turbulence in a 300-l cylindrical vessel (DESC, 2006), and Fike measured the decay of turbulence in a 2-m^3 spherical vessel with a Pitot tube technique from INERIS (Snoeys, Going, & Johnson, 2006; Snoeys, Proust, & Going, 2006). WP-1 also included a review of published work on dust explosion behaviour in linked vessels (Holbrow, 2002).

Experimental characterization of transient turbulent flows is not straightforward. Results obtained by LDA may depend on the tracer particles used, the effective sampling frequencies obtained in the experiments, and data-processing algorithms such as outlier detection criteria and smoothing procedures for isolating an 'average velocity' from the measured instantaneous velocities (Dahoe, 2000; Dahoe, Cant, Pegg, & Scarlett, 2001; Skjold, 2003). Reliable determination of turbulent length scales in transient turbulent flows is also a demanding task. Although further documentation of the relationship between turbulence data obtained with the Pitot tube technique and LDA is required, the possibility of measuring turbulence parameters in particle-laden flow, even during the course of an explosion, is interesting (Proust, 2004; Schneider & Proust, 2006; Snoeys, Going et al., 2006; Snoeys, Proust et al., 2006). High-speed videos of the dispersion process in a 300-l vessel at HSL indicated that, although it was possible to distribute the dust throughout the vessel, the resulting cloud was not homogeneous (Holbrow, 2005a). In practice, it is hardly possible to generate a perfectly dispersed dynamic dust cloud; migration of heavy particles inside turbulent eddies will result in local concentration gradients (Loth, 2000), and competition between turbulent dispersion and inelastic particle collisions will produce coherent particle swarms in the suspension (Geurts & Vreman, 2006).

2.2. Measurements of burning velocities and flame speeds

The laminar and turbulent burning velocities, S_L and S_T, denote the flame propagation velocity relative to the unreacted mixture under laminar and turbulent flow conditions, respectively. Empirical correlations between these burning velocities, and parameters describing the flow (e.g. u'_{rms} and ℓ_I), are frequently used to model turbulent premixed combustion in gaseous mixtures. Combustion modelling in DESC follows this approach, and measurements of laminar and turbulent burning velocities in various experimental configurations were therefore the main aim of WP-2. However, it is not straightforward to measure actual burning velocities (Andrews & Bradley, 1972; Dahoe, Hanjalic, & Scarlett, 2002), and in some investigations only flame propagation velocities relative to a stationary observer (i.e. flame speeds) were determined.

Fraunhofer-ICT, in cooperation with INERIS, measured burning velocities by means of the vertical open tube method (Proust, 2004; Schneider, 2006; Schneider & Proust, 2005, 2006). The apparatus consisted of a vertical channel, 1.8 m high and 0.30 m × 0.30 m square cross-section. The researchers used two different methods to generate dust clouds: either injection of dust from a pressurized dust reservoir through thin holes in pipes positioned in the corners of the channel, or sieving from the top of the channel. A chemical igniter initiated flame propagation in the lower part of the channel, and a high-speed video camera captured the speed and shape of the rising flame. Burning velocities obtained after correcting the measured flame speeds for the area of the flame surface (Andrews & Bradley, 1972) were in reasonable agreement with correlations by Bray (1990) and Gülder (1990).

Several research groups measured flame speeds in closed vessels. Zevenbergen (2004b) reported flame speed and pressure measurements performed at TU Delft in a 20-l spherical vessel fitted with an optical probe for tracking the flame front and a 1.2 Joules fused wire ignition source. However, it was not straightforward to interpret the signals from the flame probe, especially at high levels of turbulence. Holbrow (2004a) measured flame speeds and explosion pressures in a 2-m^3 autoclave at HSL. After injecting dust into an established flow field, generated by air jets from external fans, and igniting the resulting dust cloud in the centre of the vessel, thermocouples measured flame arrival times along a horizontal and a vertical axis. There measured flame speeds increased with increasing levels of turbulence, and with higher K_{St} values of the dust. However, there was significant scatter in the results, and the measured explosion pressures were significantly lower than corresponding values obtained in 20-l vessels. Holbrow (2005a) measured flame speeds and pressure development in a totally enclosed 300-l vessel, and noted that buoyancy caused the flame to expand asymmetrically. Snoeys, Going et al. (2006) and Snoeys, Proust et al. (2006) reported similar measurements in a 2-m^3 spherical vessel. Combined with reliable correlations for the decay of turbulence parameters in the larger vessels (see Section 2.1), measurements of flame speed and pressure development are valuable additions to the results obtained in 20-l vessels. Experimental data suggest that reliable quenching criteria for dust flames can be very important, especially for situations where an explosion propagates between process vessels through pipes and bends (see Section 2.6). Grosmann, Taraldset, Skjold, and Hansen (2005) described an experimental investigation by GexCon on quenching conditions for dust flames propagation through an aperture separating two enclosures. Although it was possible to identify combinations of nozzle diameters and ignition positions that resulted in certain probabilities of re-ignition in the secondary vessel, it was not possible to derive any general criteria for predicting quenching in such situations.

2.3. Dust dispersion phenomena

Dispersion of accumulated layers of combustible dust by turbulent flow or shock waves often results in escalating explosion development in coal mines or other industrial facilities. Hence, the purpose of WP-3 was to investigate, both experimentally and theoretically, the mechanisms involved in transforming dust layers into dust suspensions.

Klemens (2002–2005), Klemens and Zydak (2005), Klemens, Zydak, Kaluzny, Litwin, and Wolanski (2006), and Zydak and Klemens (2006) reported experiments performed at WUT. Dust layers were prepared along the floor of a 6.2-m long shock tube (cross section 0.072 m × 0.112 m) by a specially designed pneumatic system. After passing of the shock wave, or after the onset of turbulent flow, a technique based on attenuation of laser beams measured the increase in dust concentration at various heights above the layer. It was possible to deduce an empirical relation where dust lifting is described as injection of dust with a certain concentration, and the injection velocity is determined by parameters such as layer thickness, flow velocity above the layer, particle size, and particle density. This empirical relation imitates dust lifting in the first version of DESC. Kosinski, Hoffmann, and Klemens (2005) investigated the phenomenon of dust lifting by various mathematical techniques, including both an Eulerian–Eulerian and an Eulerian–Lagrangian approach, and showed that such modelling should account not only for the effect of the Magnus and Saffman forces, but also particle collisions.

2.4. Combustion model

The purpose of a combustion model for premixed combustion is two-fold: to define the reaction zone (i.e. the position of the flame), and to specify the rate of conversion from reactants to products (i.e. the rate of energy release). The aim of WP-4 was to develop a combustion model for turbulent dust clouds.

The flame model adopted in DESC is the same flame-thickening model used in the CFD code FLACS (FLame ACceleration Simulator), usually referred to as the β flame model (Arntzen, 1998; Kosinski, Klemens, & Wolanski, 2002). The flame thickness is about three grid cells (i.e. grid dependent), and the local burning velocity is governed by empirical correlations (Skjold, Arntzen, Storvik, & Hansen, 2005). Bradley, Chen, and Swithenbank (1988) suggested that the relationship between S_T/S_L, u'_{rms}/S_L, and the Karlovitz stretch factor K, are similar for maize starch/air and gaseous fuel/air mixtures. Bray (1990) expressed empirical data for turbulent combustion of gaseous mixtures, as summarized by Abdel-Gayed, Bradley, and Lawes (1987), in the simple equation:

$$\frac{S_T}{S_L} = 0.875\,K^{-0.392}\,\frac{u'_{rms}}{S_L}. \tag{1}$$

Arntzen (1998) reformulated this equation as $S_T = 1.81 S_L^{0.784} u'^{0.784}_{rms} \ell_I^{0.196} v^{-0.196}$, or if the kinematic viscosity v in Eq. (1) is set equal to $0.00002\,\mathrm{m^2\,s^{-1}}$ (Popat et al., 1996)

$$S_T = 15.1 S_L^{0.784} u'^{0.412}_{rms} \ell_I^{0.196}. \tag{2}$$

This is the default correlation for turbulent burning velocity in both FLACS and the first version of DESC. Whereas S_L is a well-defined and readily available parameter for many gaseous fuel–air mixtures, this is not the case for dust clouds. The approach adopted for DESC was therefore to extract estimated values for S_L from pressure–time histories measured in constant-volume explosion vessels. Whereas ISO 6184-1 (1985) specifies a 1-m^3 cylindrical vessel for determining the maximum explosion pressure $p_{\max}$ and the maximum rate of pressure rise $(\mathrm{d}p/\mathrm{d}t)_{\max}$ of dust–air mixtures, other standards also contain test procedures for the 20-l Siwek sphere (ASTM E 1226, 2000; EN 14034-1, 2004; EN 14034-2, 2006). Since most laboratories that perform tests for industry use the 20-l vessel, data from this vessel are used as the main input to the combustion model in DESC. To minimize the complications introduced by energetic ignition sources and wall effects, the analysis focus on values estimated in the inflection point of the pressure–time curve (time t_{ip} relative to onset of dispersion). An empirical equation by Dahoe, Cant, and Scarlett (2001) provides an estimate for the decay of u'_{rms} in the 20-l vessel:

$$u'_{rms}(t_{ip}) = u'_{rms}(t_0)\left(\frac{t_{ip}}{t_0}\right)^n \tag{3}$$

with the constants $u'_{rms}(t_0) = 3.75\,\mathrm{m\,s^{-1}}$, $t_0 = 0.060\,\mathrm{s}$, and $n = -1.61$; Eq. (3) is used in the range $0.060\,\mathrm{s} < t_{ip} < 0.200\,\mathrm{s}$. The corresponding empirical decay formula for ℓ_I is (Dahoe, van der Nat et al., 2001):

$$\ell_I(t_{ip}) = \ell_I(t_0)\exp\left(a_1 \ln\left(\frac{t_{ip}}{t_0}\right) + a_2\left\{\ln\left(\frac{t_{ip}}{t_0}\right)\right\}^2\right), \tag{4}$$

where a_1, a_2, $\ell_I(t_0)$, and t_0 are -3.542, 1.321, $0.012845\,\mathrm{m}$, and $0.0588\,\mathrm{s}$, respectively. A thin-flame approximation for the turbulent burning velocity yields (Dahoe, Zevenbergen, Lemkowitz, & Scarlett, 1996):

$$S_T(t_{ip}) = \frac{1}{3(p_f - p_i)}\underbrace{\left(\frac{\mathrm{d}p}{\mathrm{d}t}\right)_m V_v^{1/3}}_{K_{St}}\left(\frac{3}{4\pi}\right)^{1/3}\left(\frac{p(t_{ip})}{p_i}\right)^{-(1/\gamma)} \times\left\{1 - \left(\frac{p_f - p(t_{ip})}{p_f - p_i}\right)\left(\frac{p(t_{ip})}{p_i}\right)^{-(1/\gamma)}\right\}^{-(2/3)}, \tag{5}$$

where t_{ip} and $p(t_{ip})$ define the inflection point of the pressure–time curve, p_i and p_f are the initial and final absolute pressures, respectively, γ is the specific heat ratio, V_v is the volume of the explosion vessel, and K_{St} is the traditionally used size-corrected rate of pressure rise. An empirical relation corrects the measured overpressure p_{ex} for cooling effects to the vessel walls and the influence of pyrotechnic igniters (Cesana & Siwek, 2001):

$$p_m = \begin{cases} 5.5(p_{ex} - p_{ci})/(5.5 - p_{ci}) & \text{when } p_{ex} < 5.5\,\text{bar}, \\ 0.775 p_{ex}^{1.15} & \text{when } p_{ex} > 5.5\,\text{bar}, \end{cases} \tag{6}$$

where p_{ci} is the overpressure caused by the chemical igniter alone. A measure of laminar burning velocity follows from an inverse version of Eq. (2), using the estimated values obtained from Eqs. (3)–(5):

$$S_L(t_{ip}) = 0.0315[S_T(t_{ip})]^{1.276}[u'_{rms}(t_{ip})]^{-0.526}[\ell_I(t_{ip})]^{-0.250}. \tag{7}$$

Since chemical reactions in dust–air mixtures seldom go to completion (Lee, 1988), the combustion model requires an estimate of the mass fraction of fuel converted to products λ for various dust concentrations. In DESC, λ is determined as the fraction of the original fuel that must react with air to produce the corrected explosion pressure p_m, taking into account specific heats and heats of formation of reactants and products, and the ratio between gaseous species in reactants and products. In explosion simulations, turbulent burning velocities are found from Eq. (2), with u'_{rms} taken from the k–ε model (Section 2.5; Eq. (8)), and the integral length scale ℓ_I estimated from the algebraic expression $\tilde{\ell}_I = \min(0.025 r_F, 0.08 L_S)$, where r_F is the flame radius and L_S the minimum spatial dimension of solid boundaries surrounding the flame. Fig. 1 illustrates experimental and derived results obtained by applying the procedure described above to coal dust data from two different 20-l explosion vessels.

The empirical approach to combustion modelling has several advantages. The test procedures for the 20-l vessel are standardized, and numerous laboratories around the world use this equipment. Calibration tests are available, and, in spite of its limitations, the K_{St} value seems to provide a useful way of scaling the relative reactivity of dust samples (Cesana, 2005; Lee, 1988; Lunn, 2003). The transient flow conditions in the 20-l vessel is reasonably well documented, e.g. Dahoe, Cant, Pegg et al. (2001), Dahoe, Cant, and Scarlett (2001), Dahoe, van der Nat et al. (2001), Dahoe, Zevenbergen et al. (1996), Mercer et al. (2001), Pu (1988), Pu, Jarosinski, Johnson, and Kauffman (1990), Siwek (1977, 1988), and Skjold (2003). Furthermore, for a given dust sample, the method does not require parameters such as the volatile content, the exact chemical composition, or the particle size distribution. As for the concept of ‘maximum effective burning velocity’ (Pu, Jarosinski, Johnson, & Kauffman, 1990; Pu, Jia, Wang, & Skjold, 2006), the current approach is less sensitive to the effect of energetic ignition sources and varying turbulent flow conditions in the vessel, compared to the K_{St} value (Fig. 1). Finally, there are currently few, if any, realistic alternatives to the tests in 20-l vessels.

However, there are undoubtedly many complicating factors involved in the empirical modelling approach and further improvement and validation is required. The transient nature of the dispersion process in the 20-l vessel makes the experimental results difficult to analyse, and the effect of the dispersed phase on turbulence parameters is difficult to quantify (e.g. Dahoe, Cant, Pegg et al., 2001; Dahoe, Cant, & Scarlett, 2001; Dahoe, van der Nat et al., 2001; Skjold, 2003; Zhen & Leuckel, 1995, 1996). An 'impact mill' effect, taking place in the valve separating the dust reservoir and the 20-l vessel, alters the particle size distribution of certain types of dust significantly (Kalejaiye, 2001; Kalejaiye, Amyotte, Pegg & Cashdollar, 2006). It is not obvious that the nominal dust concentration, i.e. the weighted amount of dust divided by the volume of the vessel, is representative for the real dust concentration (Skjold, 2003). Strong ignition sources are often required for reliable ignition of highly turbulent mixtures, but the associated energy release, often distributed throughout a relatively large volume, may significantly influence both flame propagation and pressure development in the vessel (e.g. Cashdollar & Chatrathi, 1992; Going, Chatrathi, & Cashdollar, 2000; Zhen & Leuckel, 1997). The limited ranges of turbulence intensities and turbulent length scales that can be realized in the 20-l vessel differ significantly from corresponding values found in real process plants (Lee, 1988; Pu, Jarosinski, Tai, Kauffman, & Sichel, 1988). The empirical method will not work for dusts with low reactivity, since the inflection point occurs more than 0.2 s after onset of dust injection (i.e. outside the applicable range of Eqs. (3) and (4)), and turbulence production by explosion-induced flow may influence the estimated turbulence parameters for highly reactive dust–air mixtures. The assumption of a thin spherical flame, used in the derivation of Eq. (5), is not compatible with significant flame thickness (or volumetric combustion); a possible solution involves fitting an integral balance model to the measured pressure–time curve (Dahoe, Zevenbergen et al., 1996), but this approach is somewhat limited since it requires a relatively weak ignition source. Furthermore, the alleged agreement between the K_{St} and $p_{\max}$ values obtained in the 1-m^3 ISO vessel and the 20-l Siwek sphere is questionable (Proust, Accorsi, & Dupont, 2006). Finally, it has proven rather difficult to obtain reliable data on thermodynamic properties for powders; a possible solution involves using the 20-l vessel as a calorimeter, but it may not be straightforward to perform reliable temperature measurements.

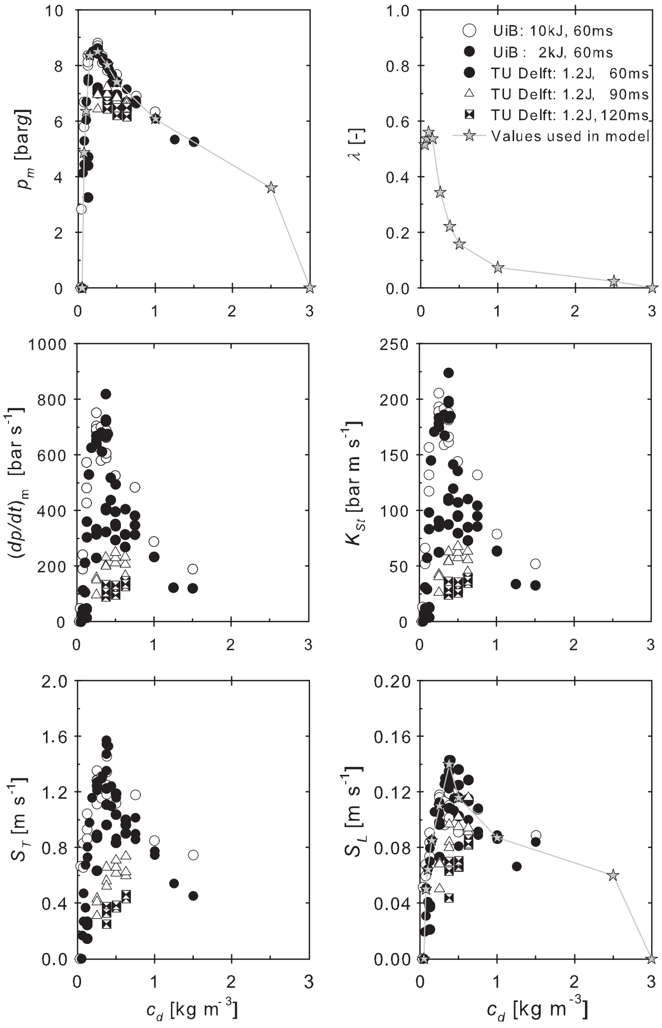

Fig. 1. Experimental values for p_m, λ, $(dp/dt)_m$, K_{St}, S_T, and S_L for the coal dust used in the DESC project: data from UiB and TU Delft (Zevenbergen, 2004b); measured lower flammability limit 50 g m^{-3}, and upper flammability limit arbitrary set to 3000 g m^{-3}.

Improvements and further validation of the combustion model in DESC are also required, especially a thorough experimental validation of the correlations for turbulent burning velocity in dust clouds; this could involve tests in closed vessels, vertical tubes, burners, and channels with repeated obstacles (e.g. Dahoe, Hanjalic et al., 2002; Pu, 1988; Pu, Mazurkiewicz, Jarosinski, & Kauffman, 1988; Schneider & Proust, 2005). Further work must also focus on improving the models for non-zero slip velocity between particles and fluid, flame thickness and volumetric combustion, and turbulent quenching of dust flames (e.g. Gieras, Glinka, Klemens, & Wolanski, 1995; Lee, 1988). Further efforts to decrease the grid sensitivity of the simulations, especially during the initial phase of flame propagation (governed by subgrid models), are also required (Skjold, Pu, Arntzen, Hansen, Storvik, Taraldset et al., 2005); results from balloon experiments could prove useful to achieve this goal (Skjold & Eckhoff, 2006). Finally, there are unresolved issues concerning the effect of suppression agents like sodium bicarbonate on the combustion process, thermodynamic relations for non-organic materials (e.g. metals), and criteria for quantifying the likelihood of deflagration to detonation transition (DDT) in dust–air mixtures.

2.5. Development of the CFD code

The purpose of WP-5 was to develop the CFD code. Since the graphical user interfaces and most of the numerical schemes were adopted from the existing CFD code FLACS for gas explosions, the two codes have many features in common (Skjold, Arntzen, Storvik et al., 2005). Both are finite-volume CFD codes where transport equations for mass, momentum, enthalpy, fuel, mixture fraction, turbulent kinetic energy k, and rate of dissipation of turbulent kinetic energy ε are solved on a structured Cartesian grid. All solid objects are mapped to the grid using porosities, and sub-grid models are used to describe phenomena that cannot be resolved on the grid. Simulation scenarios, including geometry, grid, initial and boundary conditions, time, and position of ignition, monitor points, pressure relief panels, output parameters, etc., are defined in the pre-processor CASD (Computer Aided Scenario Design), and results from simulations are presented in the post-processor Flowvis. Compressible flow is solved by the SIMPLE algorithm (Patankar, 1980), and both codes have first-order backward Euler time differencing schemes, second-order upstream and central differencing schemes for convective fluxes, second-order central differencing scheme for diffusive fluxes, and conjugant gradient solvers. To achieve independent and rapid build-up of the turbulent flow field and representative turbulence production from objects not resolved by the computational grid, the standard k–ε turbulence model (Lauder & Spalding, 1974) is modified by adding source terms for turbulence production by velocity gradients (Arntzen, 1998). The model estimates u'_{rms} and ℓ_I from the expressions:

$$u'_{rms} = \left(\frac{2}{3}k\right)^{1/2} \tag{8}$$

and

$$\ell_I = C_I \frac{k^{3/2}}{\varepsilon}, \tag{9}$$

respectively, where C_I is 0.202 (Abdel-Gayed & Bradley, 1981).

The modelling of particle-laden flow in DESC is quite simple. It treats the dust cloud as an equilibrium mixture where dispersed particles are in dynamic and thermal equilibrium with the gaseous phase (e.g. Crowe, Sommerfeld, & Tsuji, 1998; Marble, 1970). This corresponds to Eulerian approach in the limiting case when the Stokes number approaches zero. A Stokes number based on the integral time scale of turbulence quantifies the deviations from the above assumption for a given particle size:

$$St_I = \frac{\tau_p}{\tau_I} \approx \left(\frac{\rho_p d_p^2}{18\mu_f}\right)\left(C_I \frac{k^{1.5}}{\varepsilon\, u'_{rms}}\right)^{-1}, \tag{10}$$

where τ_p is the particle response time, τ_I the integral time scale of the flow, ρ_p is the particle density, d_p a characteristic particle size, and μ_f the dynamic viscosity of the fluid. Small Stokes numbers (<0.01) imply particles that follow the fluctuating flow, while particles with large Stokes numbers (>100) do not respond significantly to turbulent velocity fluctuations. To facilitate simulation of explosion suppression systems, DESC contains a transport equation for a second mixture fraction.

The current modelling of particle-laden flows in DESC has some inherent limitations, and improvements in future versions may include more realistic modelling of multiphase flow by introducing either an Eulerian–Eulerian or an Eulerian–Lagrangian description of the gaseous and solid phases. Although the Cartesian grid system is robust and a well-established technology, other grid systems may prove to be better suited for representing complex internal geometries. To continuously identify and replace the weakest models is an essential activity for anyone involved in developing CFD codes for complex phenomena like industrial gas and dust explosions.

2.6. *Validation of the CFD code*

Experimental data are required for the validation of any CFD code. For codes intended for process safety applications, comparison with existing design methodology may also be relevant. Hence, main tasks in WP-6 included dust explosion experiments in connected vessel systems, simulating experimental dust explosions reported in literature, comparing predictions by CFD and existing guidelines for explosion venting, and measurements of flow and dust concentrations in process plants.

The validation work performed by GexCon focused on simulating dust explosion experiments described in literature. Skjold, Arntzen, Hansen, Storvik, and Eckhoff (2006) and Skjold, Arntzen, Hansen, Taraldset et al. (2005) presented results obtained with DESC 1.0b2, indicating a reasonably good agreement with experimental data obtained in relatively simple geometries such as silos (Eckhoff, Fuhre, & Pedersen, 1987; Hauert, Vogl, & Radandt, 1996) and interconnected vessel systems (Lunn, Holbrow, Andrews, & Gummer, 1996). Skjold, Pu et al. (2005) simulated flame acceleration experiments with gas (methane) or dust (maize starch) reported by Pu (1988) and Pu et al. (1988). The results revealed that the simulated flame propagation was sensitive to grid resolution, particularly during the initial phase controlled by subgrid models. Earlier work on dust explosion modelling with FLACS and DESC is described by van Wingerden (1996), van Wingerden, Arntzen, and Kosinski (2001), Arntzen, Salvesen, Nordhaug, Storvik, and Hansen (2003), Siwek et al. (2004), and Hansen, Skjold, and Arntzen (2004).

Skjold and Hansen (2005) applied the empirical approach outlined in Section 2.4 to experimental data obtained for either propane–air or dust–air mixtures in a 20-l explosion vessel. The methodology involved igniting the turbulent fuel–air mixtures to deflagration at various ignition delay times, and estimating u'_{rms}, ℓ_I, S_T, and S_L from Eqs. (3)–(5) and (7). Figs. 2 and 3 show estimated turbulent and laminar burning velocities as a function of u'_{rms} for gaseous and dust–air mixtures, respectively. Although there is considerable scatter in the results, S_T

values for propane (Fig. 2) are within the range predicted by Eq. (1), whereas values for the dusts (Fig. 3) show a more linear dependence on u'_{rms}. Assuming Eqs. (3)–(5) and (7) valid, the estimated laminar burning velocities in Figs. 2 and 3 should assume constant values for a given fuel concentration. However, the values for propane decrease with increasing u'_{rms} for all concentrations, while the values for both dusts increase somewhat. Although these results indicate that correlations for turbulent burning velocity may differ for gases and dusts, other mechanisms, such as a higher degree of volumetric combustion in dust–air mixtures, or the influence of the dispersed particles and/or combustion on the decay of turbulence inside the 20-l vessel, may also influence the results.

Klein, van der Voort, and Versloot (2005) and Klein, van der Voort, van Zweden, and van Ierschot (2005) reported flame speed measurements from medium-scale explosion tests performed in a closed vessel system at TNO. The apparatus consisted of two 1-m^3 explosion vessels connected by pipes of various lengths, with and without obstructions or a 90° bend in the pipe. Klein et al. also considered the effect of dust type (coal, potato starch, and silicon), ignition position, and venting of one of the vessels. For all dust types, the introduction of either a bend, or obstacles in the connecting pipe, resulted in delayed jet ignition in the secondary vessel, and hence increased pressure piling.

Holbrow (2004b, 2005b, 2005c) reported work performed by HSL on large-scale explosions in a system consisting of two cylindrical vented vessels, 20 and 2 m^3, connected by a pipe (0.50 or 0.25 m in diameter) with a sharp 90° bend (Fig. 4). After dust injection from four external 2.3-l pressurized reservoirs, one in the 2-m^3 vessel and three in the 20-m^3 vessel, the suspensions were ignited in the larger vessel by electric fuse heads and 25 g of black powder (about 50 kJ). Pressure transducers (channels 1–6) were located in both vessels and in the pipe, and thermocouples (channels 7–14) measured flame speed along the centre-line of the pipe. The experimental programme included 26 regular tests with four types of dust (coal, silicon, and two types of potato starch). Explosions transmitted more readily through the 0.50 m diameter pipe than through the 0.25 m diameter pipe, and explosions involving potato starch were more likely to transmit to the 2-m^3 vessel than the more reactive coal dust. When no transmission occurred, the flame extinguished close to the 90° bend. Fig. 5 illustrates experimental and simulated results from the only test that produced a significant pressure enhancement in the secondary vessel, i.e. test no. 13 with coal dust (K_{St} 150 bar m s^{-1}). Poor repeatability, and the fact that none of the other 25 tests produced significant pressure enhancement in the secondary vessel, represents a significant challenge for the validating of the CFD code. Except from three tests (no. 12, 13, and 15, with pressures 0.8, 2.9, and 1.2 bar, respectively), the maximum overpressures measured in the 2-m^3 vessel were in range 0.02–0.35 bar.

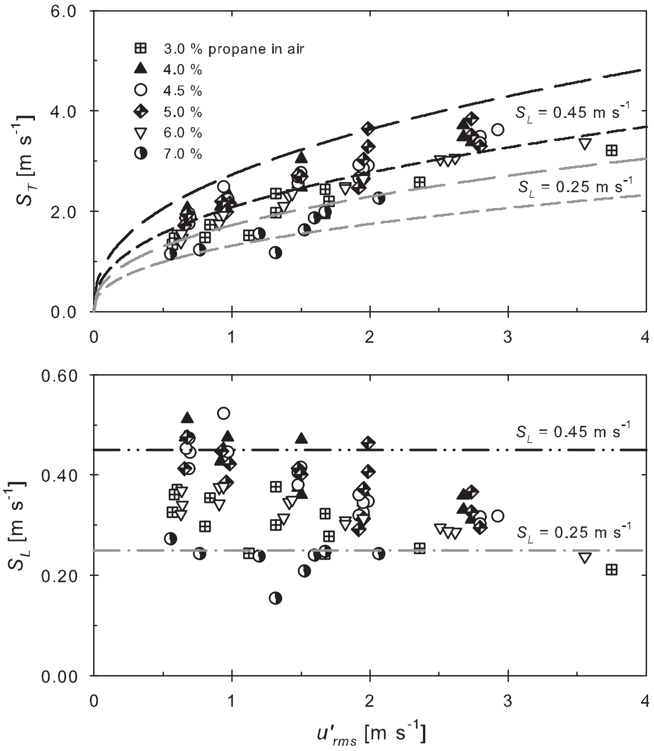

Fig. 2. Estimated turbulent and laminar burning velocities for propane–air mixtures. S_T predicted by Eq. (2) for typical values of S_L (0.25 and 0.45 m s^{-1}) and ℓ_I (1 mm short dashed lines; 4 mm long dashed lines) are included in the top figure.

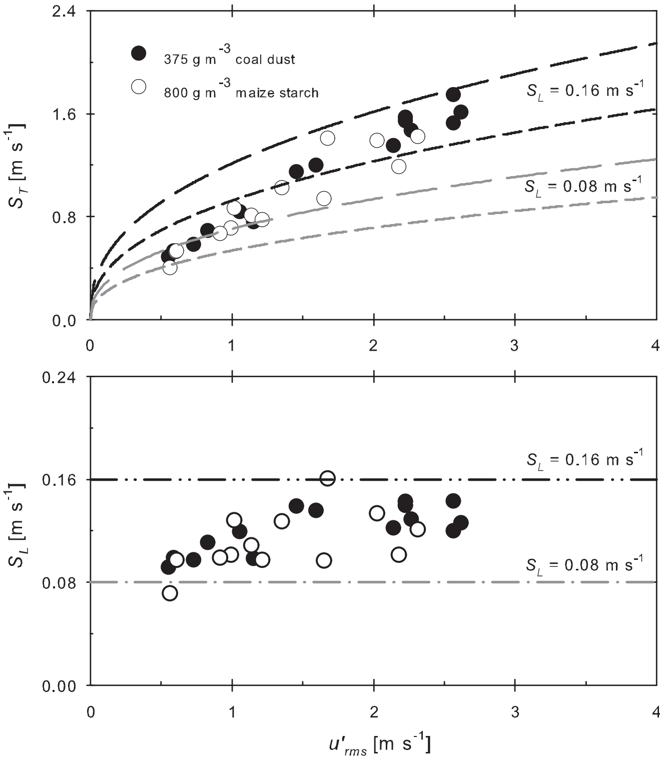

Fig. 3. Estimated turbulent and laminar burning velocities for two dust–air mixtures. S_T predicted by Eq. (2) for typical values of S_L (0.08 and 0.16 m s^{-1}) and ℓ_I (1 mm short dashed lines; 4 mm long dashed lines) are included in the top figure.

The results from both TNO and HSL suggest that turbulence production and quenching effects caused by bends in the connecting pipe can have significant influence on flame propagation and pressure build-up in interconnected vessel systems. However, it is not straightforward to include models for quenching in a CFD code, and at the same time ensure that the results from the simulations are on the conservative side in most practical situations. Experiments by Vogl and Radandt (2005) show that explosions involving dusts of relatively low reactivity (wheat flour, K_{St} 100 bar m s^{-1}) can propagate through a 12-m-long pipe with diameter 27 mm. Vogl and Radandt noted that the expansion flow of hot combustion products from the primary vessel had a dominant influence on the observed flame speeds.

Inburex simulated vented dust explosions in various vessel configurations, and compared the results with experimental data and recommendations from existing design guidelines (Rogers & Coupin, 2005). Although the

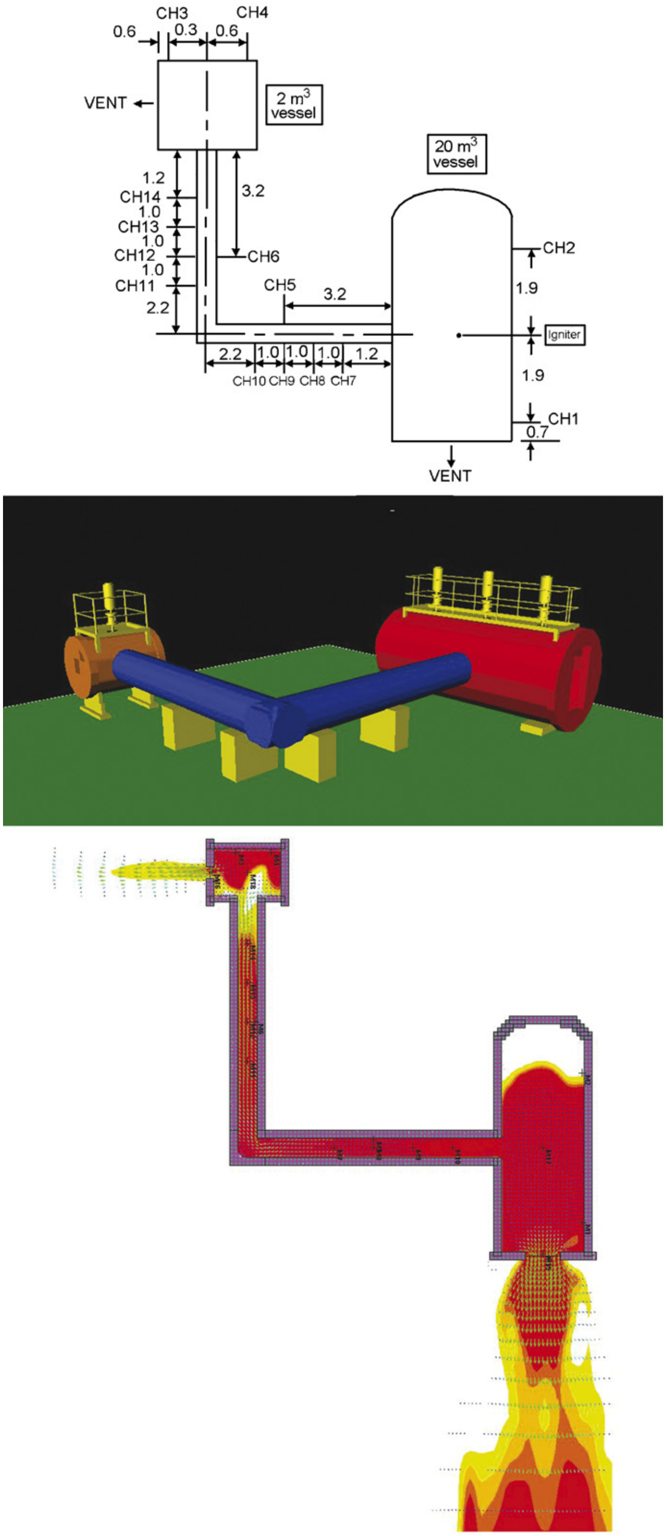

Fig. 4. Schematic of the interconnected vessel system at HSL (top, from Holbrow, 2004b); DESC representation of the same geometry (middle); and a cross-section illustrating simulated flame development in the system (bottom).

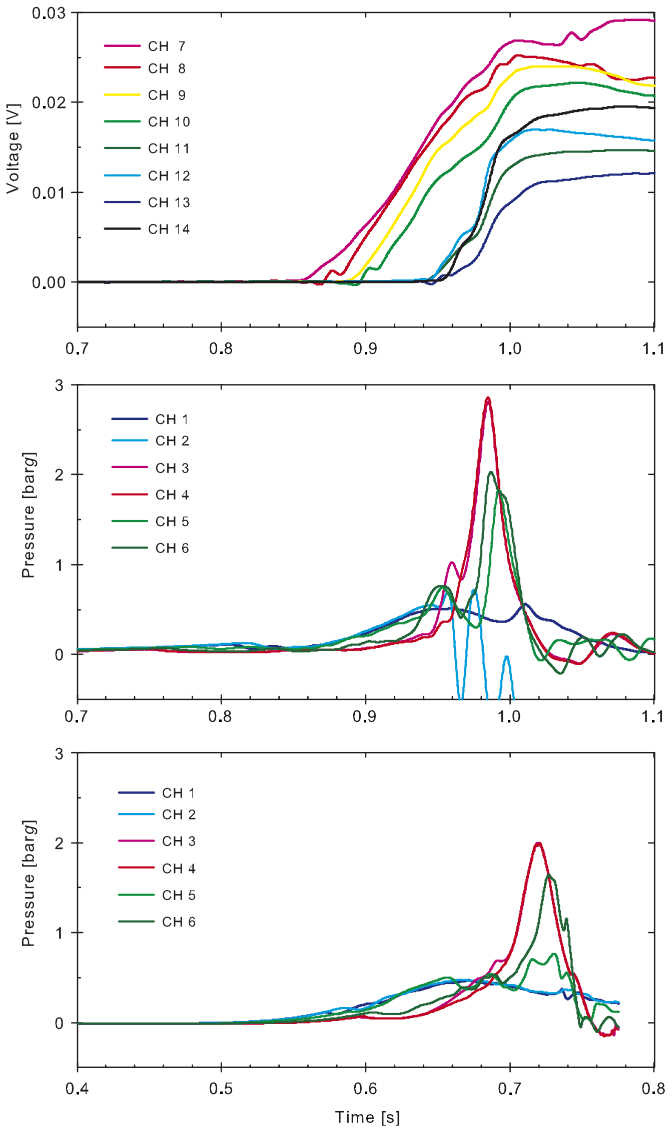

Fig. 5. Experimental and simulated results from test no. 13 (coal dust) in the interconnected vessel system (Fig. 4): measured flame arrival at the thermocouples (top) and pressure development (middle – notice that the pressure sensor CH2 dropped out after about 0.95 s), and pressure development simulated with DESC (bottom).

DESC code simulated the general course of dust explosions reasonably well, improved accuracy would be required to achieve a level suitable for design purposes. FSA measured dust concentrations and flow parameters in typical powder-handling units under normal process conditions (Shi, Arnold, Vogl, & Radandt, 2005a, 2005b). Such data are valuable for validation purposes, and when selecting appropriate initial conditions for CFD simulations.

Experimental data of high quality are required for further validation of DESC and other CFD codes for dust explosion modelling. In an ideal experimental setup for validation purposes, simultaneous measurements of the relevant turbulence parameters, actual dust concentrations, flame temperatures, burning velocities, flow velocities, etc., in several positions, through series of repeated tests, would yield the necessary data. However, in practice, both the lack of reliable measuring techniques, and the limited repeatability of large-scale dust explosion experiments, cause problems. Comparative studies of flame propagation and pressure build-up in dust clouds and gaseous mixtures, starting from similar initial conditions, may produce valuable results.

2.7. *Software package and exploitation of results*

The main objective of WP-7 was to prepare a complete software package, comprising the validated CFD code and appropriate user documentation. Partners in the DESC consortium presented results from the project at the ESMG Symposium in Nürnberg, 11–13 October 2005, including a fully functional *beta* version of the code. GexCon released the first official version (DESC 1.0) in June 2006. DESC users are obliged to attend a compulsory training course, and have the option of attending regular user group meetings. Although DESC 1.0 only runs under the Linux operating system, future releases will also be available on other platforms.

3. Discussion and conclusions

Dust explosions can cause great material damage, injury, and loss of life. Current guidance on explosion protection originates from experiments performed in relatively simple vessel arrangements, and is not necessarily applicable when explosions propagate through complex industrial plants. The main aim of the DESC project was therefore to develop a simulation tool based on CFD that could predict the potential consequences of industrial dust explosions. The overall approach adopted to achieve this goal was to combine the development of the CFD code with experimental work covering a broad range of relevant topics. Although the initial ambitions were somewhat adjusted in the course of the project, the experimental programme nevertheless resulted in many useful results, and the modelling work produced a commercially available CFD code for dust explosions. Hence, the DESC project represented a valuable continuation of earlier work on dust explosion safety in Europe (e.g. Gibson, 1996), and an important step forward for general process safety in powder-handling plants worldwide.

Several aspects of the modelling in DESC require further work, including the representation of particle-laden flow, the applicability of general correlations for turbulent burning velocity in describing flame propagation in dust clouds, and the lack of reliable physical models for quenching and re-ignition phenomena in dust flames. Poor repeatability and many unresolved issues associated with experimental dust explosion research represent a major challenge for future validation work (e.g. Eckhoff, 2003; Holbrow, 2005c). Although the required accuracy of such measurements is less stringent for safety analysis, as long as the values are conservative, improved and standardized test methods would be most welcome.

The motivation for introducing a CFD code for dust explosions is not to replace existing standards and guidelines for process safety design (e.g. EN 14373, 2005; EN 14460, 2006; EN 14491, 2006; prEN 15089, 2004; NFPA 68, 2007), but rather to complement these by offering a way of predicting the outcome of complex explosion scenarios not covered by existing methodology (Lunn, 2005; Zalosh, 2006). Results from a properly validated CFD code will be valuable for risk assessments in powder-handling plants, thereby fulfilling essential health and safety requirements of recent EU Directives (ATEX 1999/92/EC, 1999; ATEX 94/9/EC, 1994). Potential users of such codes could be explosion consultants, engineers in the powder-handling industry, or regulatory authorities. Unlike the offshore oil and gas industry (e.g. NORSOK, 2001), there is currently no established practice or guidelines for the use of CFD tools during risk assessments in powder-handling plants. It nevertheless seems reasonable to adopt a 'realistic worst case' approach when dealing with dust explosions (Hansen, Skjold, & Storvik, 2005; Skjold et al., 2006), since design based on actual process conditions may be of limited value. Accidental dust explosions often occur during abnormal process conditions, e.g. during start-up or shut-down of plants, and re-dispersion of accumulated dust layers inside process units can increase the actual dust concentration significantly beyond the 'nominal concentration' (e.g. mass production rate of dry powder divided by volumetric flow rate of air). Although a relatively conservative approach was sought in the first version of DESC, regarding both the choice of implemented models, and guidelines for users, effects caused by phenomena that are not properly modelled, such as turbulent quenching, are inherently difficult to predict. Whereas consequence assessments based on CFD simulations are useful when optimizing explosion mitigation systems in powder-handling plants, especially during the design phase, risk reduction should still primarily focus on preventing accidents from taking place.

CFD can increase our understanding of dust explosions at various levels. Detailed studies of single particle combustion, laminar burning velocity, dust lifting, etc.

are of vital importance for understanding the underlying physical and chemical phenomena. However, reliable correlations between parameters such as S_T, S_L, u'_{rms}, and ℓ_I are of paramount importance for flow solvers addressing the actual industrial hazard—transient turbulent reacting multiphase flow through complex geometries. Our current understanding of the dust explosion phenomenon is limited, and the use of CFD codes to predict the outcome of explosion scenarios in powder-handling plants is still in its infancy. Hence, the following statement by Bardon and Fletcher (1983) still holds good:

> "*There remains much to be done before dust explosions are adequately understood.*"

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