Flame propagation in dust clouds

Numerical simulation and experimental investigation

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Abstract

This dissertation describes the development and validation of a methodology for estimating the consequences of accidental dust explosions in complex geometries. The approach adopted entails the use of results from standardized tests in 20-litre explosion vessels as input to the combustion model in a computational fluid dynamics (CFD) code, and the subsequent validation of the model system by comparing with results from laboratory and large-scale experiments. The PhD project includes dedicated laboratory experiments designed to explore selected aspects of flame propagation in dust clouds, and to reveal similarities and differences between flame propagation in gaseous mixtures and mechanical suspensions of combustible powder in air.

The research project represents a continuation of numerous efforts by various research groups, where the key underlying problem has been the scaling of results obtained in laboratory tests for predicting the consequences of dust explosion scenarios in industry. The traditional approach to the scaling problem entails the use of empirical correlations, typically represented as nomographs or formulas in relevant safety standards. It is generally accepted that empirical correlations may work reasonably well for simple geometries, such as isolated process vessels and silos. The need for more sophisticated methods arises for accident scenarios that involve complex geometrical boundary conditions, such as flame propagation in connected vessel systems and secondary dust explosions inside buildings.

The European Commission (EC) supported the Dust Explosion Simulation Code (DESC) project under the Fifth Framework Programme. The goal was to develop and validate a CFD code for simulating industrial dust explosions in complex geometries. To this end, GexCon created the CFD code DESC (Dust Explosion Simulation Code)[1] by modifying the existing CFD code FLACS (FLame ACceleration Simulator), originally developed for simulating gas explosions in congested offshore geometries. The specific contributions from the candidate with respect to the development of the CFD software is limited to the methodology for estimating combustion parameters for a given dust sample from experimental results, the validation of the resulting model system against experimental data, and general participation in the R&D team during the development process.

The modelling of particle-laden flow and heterogeneous combustion in the CFD code DESC involves several simplifying assumptions. The flow model assumes thermal and kinetic equilibrium between the dispersed particles and the continuous phase, and the k-ε turbulence model in FLACS remains unchanged for multiphase flows. The empirical correlation for the turbulent burning velocity in dust clouds originates from experiments with premixed combustion in gaseous mixtures. The fraction of dust that takes part in the combustion reactions, as function of the nominal dust concentration, is estimated from the explosion pressures measured in a constant volume explosion vessel. The thermodynamic data available in FLACS limit the application area to materials containing the elements carbon, hydrogen, oxygen, nitrogen and sulphur. The simplifications limit the application area of DESC to certain classes of materials, and flame propagation in dust clouds with relatively high reactivity. DESC do not contain models for simulating phenomena such as agglomeration, gravitational settling, and selective separation of particles in flow through cyclones or along other curved paths.

In spite of the simplicity of the model system, the results from the validation work show that the CFD code DESC can describe the course of dust explosions in relatively complex geometries with reasonable accuracy relative to the inherent spread in the experimental results. The results obtained for silo explosions reproduce trends observed for variation in vent area and ignition position from various experiments. Results obtained for flame propagation sustained by dust dispersion from a layer indicate that the empirical model for dust lifting in DESC is suitable for the purpose. Results obtained for dust explosions vented through ducts reproduce the experimental trends fairly well. Simulations of dust explosions in a system of two vented vessels connected by a pipe with a 90° bend indicate that the DESC can reproduce relatively complex chains of events, including dust lifting from a layer. The

[1] GexCon recently changed the name of the CFD code DESC to FLACS-DustEx.

results for the connected vessel system also demonstrate how sensitive the results can be with respect to modest changes in the initial and boundary conditions. Finally, simulations of explosion experiments in elongated vessels with repeated obstacles reproduce the experimental trends fairly well.

Although the results from the validation work indicate that CFD simulations can become a valuable tool for consequence modelling and design of industrial facilities, the modelling in DESC requires further improvements. An essential improvement entails fundamental changes to the numerical solver to reduce in the influence of the grid resolution on the results from the simulations. In the current versions of FLACS and DESC, simulation of explosion scenarios is subject to strict grid guidelines. The current versions of both codes use a structured Cartesian grid, with limited possibilities for local grid refinement. This poses a particular challenge for DESC, since the grid resolution required to resolve complex internal geometries on a structured Cartesian grid varies significantly from case to case. The long-term solution to these challenges will presumably entail the use of adaptive mesh refinement (AMR), and this is outside the scope of the present work.

The model system may also benefit from various other improvements, such as turbulent burning velocity correlations specifically developed for dust explosions, an explicit model for turbulent flame thickness, radiation models, local grid refinement in the region where ignition occurs, reduced dependence on empirical input to the model system, and in general more realistic modelling of particle-laden flow and heterogeneous combustion. There is, however, a fine balance between the level of detailed information that must be specified in the model, and the applicability and user-friendliness of the model system. For most industrial applications of a CFD tool for dust explosions, there are significant inherent uncertainties associated with initial and boundary conditions.

Dust explosion experiments in transparent balloons show that the initial phase of flame propagation in turbulent dust clouds can progress in a distributed manner, with very limited energy output. This observation may explain some of the challenges associated with the analysis of pressure-time histories from 20-litre explosion vessels for dust explosions when using a weak ignition source. Experiments in a 3.6-m flame acceleration tube demonstrate the importance of explosion-generated turbulence for dust explosions, and illustrate the challenge associated with poor repeatability in dust explosion experiments. The results obtained for propane-air mixtures in the same apparatus indicate that FLACS under-predicts the rate of combustion for turbulent flame propagation in fuel-rich propane-air mixtures.

The CFD code DESC represents a significant step forward for process safety related to dust explosions in the process industry. There is, however, significant room for further improvements to the model system, and dedicated experiments will play an important role for the future development of the code. Improved safety in the process industry requires reliable and well-documented consequence models, and future development of DESC should include an integrated framework for model validation, including verification and testing.

Scientific environment

The *philosophiae doctor* (PhD) project started in January 2004. The work progressed under the principal supervision of Professor Rolf K. Eckhoff at the University of Bergen (UiB), Faculty of Mathematics and Natural Sciences, Department of Physics and Technology (IFT), Research Group for Petroleum and Process Technology, Section for Process Safety Technology; Dr. Bjørn J. Arntzen (IFT and GexCon) was co-supervisor.

The candidate has been an employee in the research and development (R&D) department at GexCon AS since November 2003 – initially as project manager, and since July 2008 as department manager (R&D Director). GexCon R&D develops the computational fluid dynamics (CFD) code FLACS (FLame ACceleration Simulator), including DESC. The CFD code DESC (Dust Explosion Simulation Code) is part of the commercial CFD code FLACS[2]. The development of FLACS started at Chr. Michelsen Institute (CMI) in 1980, continued at Christian Michelsen Research (CMR) from 1992 to 2000, and is currently the primary R&D activity at GexCon AS. CMI initiated GexCon, 'Gas Explosion Consultancy', in 1987, and CMR established GexCon AS, 'Global Explosion Consultants', in 1998. GexCon AS is a wholly owned subsidiary of CMR. The shareholders of CMR are UiB (50%), Uni Research AS (35%), Statoil New Energy AS (5%), Sparebanken Vest (5%) and CGG Veritas Services Norway AS (5%).

The development of the CFD code FLACS, including DESC, is a team effort within GexCon R&D. As of June 2014, the R&D department has14 full-time and three part-time employees, of which eight hold PhD degrees and three currently pursue PhDs: the candidate and two industry-PhDs supported by the Research Council of Norway (RCN).

Development, testing and validation of the CFD code DESC represent a significant part of the PhD project. The European Commission (EC) supported the DESC project under the Fifth Framework Programme. The project started in January 2002 and ended in June 2006. The Health and Safety Laboratory (HSL) coordinated the DESC project, and GexCon was one of the partners in the consortium. The author has not worked directly on the source code for the CFD software, but has contributed with input to the implemented models, and been responsible for the testing and validation work related to DESC. The author has organized training courses and workshops for users of the software, organized DESC User Group meetings, and used DESC in consultancy projects for industry.

The author conducted most of the small-scale experiments in a 20-litre vessel at the Dust Explosion Laboratory at IFT (Skjold, 2003), and the experiments in transparent balloons and in the 3.6-metre flame acceleration tube (FAT) in the laboratories at GexCon. The Mechanical and Electrical Workshops at IFT contributed significantly to the construction of the experimental equipment. Several MSc and PhD students from various universities took part in the experiments. The work on the PhD project included significant interaction with the global research community in the field of dust explosions, in projects as well as international meetings and conferences, resulting in several joint publications. GexCon and UiB hosted the Tenth International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosions (X ISHPMIE) in Bergen on 10-14 June 2014. The symposium included the Sixteenth International Colloquium on Dust Explosions.

The candidate financed most of the PhD project, but the European Commission, IFT, Karmsund Maritime AS (previously Kopervik Slip AS), Aibel AS (Aibel Haugesund), Statoil ASA, Os Transformatorfabrikk AS and GexCon AS supported the project by various means.

[2] GexCon recently changed the name of the CFD code DESC to FLACS-DustEx. GexCon owns all intellectual property rights to the CFD code FLACS™.

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I want to thank all past and present colleagues at *GexCon R&D* for their valuable contributions. The generous help and guidance from *Idar E. Storvik*, *Olav R. Hansen*, *Ole Jacob Taraldset* and *Jens A. Melheim* were particularly helpful during the PhD project. Contributions from other colleagues at GexCon have also been most helpful, in particular the advice and encouragement from Dr. *Kees van Wingerden*, and the technical assistance from the team at *GexCon Labs*. Special thanks are also due to several individuals at *University of Bergen* (UiB), *Department of Physics and Technology* (IFT), all of whom showed special interest in the project: *Kåre Slettebakken*, *Leif Egil Sandnes*, *Svein Midtun* and *Roald Langøen* at the Mechanical Workshop at IFT, *Werner Olsen* at the Electronic Laboratory at IFT, and *Grete Kvamme Ersland*, *Simone Katharina Heinz*, *Jan Petter Hansen*, *Geir Anton Johansen* and *Terje Finnekås* from the Administration at IFT.

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List of publications

This thesis describes the work presented in the following 13 publications:

A Skjold, T., Arntzen, B.J., Hansen, O.R., Taraldset, O.J., Storvik, I.E. & Eckhoff, R.K. (2005). Simulating dust explosions with the first version of DESC. *Process Safety and Environmental Protection*, **83**: 151-160. ISSN: 0957-5820. DOI: http://dx.doi.org/10.1205/psep.04237

B Skjold, T., Arntzen, B.J., Hansen, O.J., Storvik, I.E. & Eckhoff, R.K. (2006). Simulation of dust explosions in complex geometries with experimental input from standardized tests. *Journal of Loss Prevention in the Process Industries*, **19**: 210-217. ISSN: 0950-4230. DOI: http://dx.doi.org/10.1016/j.jlp.2005.06.005

C Skjold, T., Pu, Y.K., Arntzen, B.J., Hansen, O.J., Storvik, I.E., Taraldset, O.J. & Eckhoff, R.K. (2005). Simulating the influence of obstacles on accelerating dust and gas flames. *Twentieth International Colloquium on the Dynamics of Explosions and Reactive Systems* (ICDERS), Montreal, 31 July - 5 August 2005: 5 pp.

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I Skjold, T. (2010). Flame propagation in dust clouds: challenges for model validation. *Eighth International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions* (ISHPMIE), Yokohama, 5-10 September 2010: 11 pp.

J Skjold, T. (2014). Simulating vented maize starch explosions in a 236 m^3 silo. *Eleventh International Symposium on Fire Safety Science*, University of Canterbury, New Zealand, 10-14 February 2014, International Association for Fire Safety Science (IAFSS): 12 pp.

K Castellanos, D., Skjold, T., van Wingerden, K., Eckhoff, R.K. & Mannan, M.S. (2013). Validation of the DESC code in simulating the effect of vent ducts in dust explosions. *Industrial & Engineering Chemistry Research*, **52**: 6057-6067.
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L Skjold, T., Olsen, K.L. & Castellanos, D. (2013). A constant pressure dust explosion experiment. *Journal of Loss Prevention in the Process Industries*, **26**: 562-570. ISSN: 0950-4230. DOI: http://dx.doi.org/10.1016/j.jlp.2012.08.003

M Skjold, T., Castellanos, D., Olsen, K.L. & Eckhoff, R.K. (2014). Experimental and numerical investigations of constant volume dust and gas explosions in a 3.6-m flame acceleration tube. Journal of Loss Prevention in the Process Industries, 30: 164-176. ISSN: 0950-4230.
DOI: http://dx.doi.org/10.1016/j.jlp.2014.05.010

The published papers will be reprinted with permission from *Institution of Chemical Engineers* (papers A, D and E), *Elsevier* (papers B, H, L and M), *University of Edinburgh* (Paper F), *International Association for Fire Safety Science* (Paper J) and *ACS Publications* (Paper K). The author holds the copyright for papers C, G and I.

The following publications are not included in the dissertation, for the sake of brevity:

- Hansen, O.R., Skjold, T. & Arntzen, B.J. (2004). DESC – a CFD-tool for dust explosions. *International ESMG Symposium*, Nuremberg, Germany, 16-18 March 2004, European Safety Management Group (ESMG), ISBN: 3-9807567-3-4: 13 pp.

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Table of contents

1. Introduction

1.1 Outline

This dissertation consists of 13 publications that address the hazard posed by accidental dust explosions from the perspective of process safety and risk management, with particular emphases on quantitative consequence modelling and safe design of industrial facilities. The work entails numerical simulations and experimental investigations of turbulent flame propagation in dust clouds. This chapter introduces some basic concepts and definitions, elaborates on the motivation and background for the work, and summarizes the modelling approach. Chapter 2 summarizes the publications, and Chapter 3 highlights the main conclusions and provides suggestions for further work.

1.2 Risk management

Figure 3 shows a schematic representation of the various aspects of risk management. Risk management refers to a coordinated set of activities and methods used to direct an organization and to control the risks that can affect its ability to achieve its objectives (Aven & Vinnem, 2007; Vinnem, 2014). Management of operational risk should take into account previous events and near misses, safety barriers, modifications and ageing of installations, technological developments, the likelihood of natural disasters, safety training and risk awareness, etc. The ALARP principle implies that the operators of a facility should reduce the risk to a level 'as low as reasonably practicable'.

The purpose of risk analysis and risk assessment is to systemize knowledge and uncertainties about phenomena, processes and activities in a system, to describe and discuss the results of the analysis in order to provide a basis for evaluating what is tolerable and acceptable, and to compare different design options and risk reducing measures (Aven & Vinnem, 2007). Quantitative risk assessment (QRA) has proven particularly valuable for detecting deficiencies and improving safety performance in complex technical systems. However, a qualitative approach may suffice for simpler systems.

There are inherent uncertainties associated with most risk assessments: the hazard identification process is rarely complete, there may be insufficient data to support precise estimates of the event frequencies, and there can be significant uncertainty associated with the estimates for the consequences of hazardous events. The main uncertainties associated with the consequences of flow-related accident scenarios, including dust explosions, relate to scaling and complexity. The solution to a given flow problem depends on the initial and boundary conditions, e.g. the initial flow field and the geometry. This poses inherent limitations to the applicability of empirical correlations for non-trivial systems.

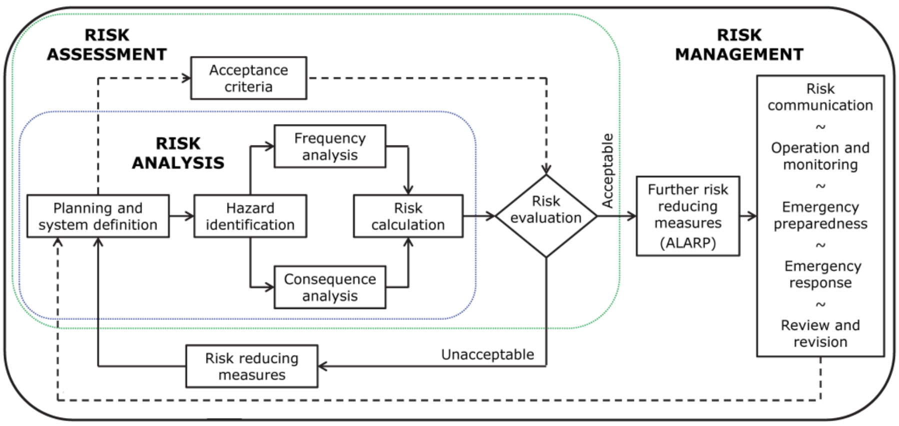

Figure 1: Schematic representation of risk analysis, risk assessment and risk management.

1.3 Dust explosions

This section provides a brief introduction to dust explosions.

1.3.1 The hazard

Accidental dust explosions have caused severe material damage, injuries, and loss of life in the process and mining industries (Price & Brown, 1922; Bartknecht, 1993; Eckhoff, 2003; Mannan, 2012; Amyotte, 2013). Figure 2 illustrates the explosion pentagon for fuel-air explosions (Kauffman, 1981). Dust explosions pose a hazard whenever combustible solid material is present in the form of fine powder, there is a possibility of dispersing a sufficient mass of the material in air to form an explosive dust cloud within a relatively confined and/or congested volume, and there is an ignition source present.

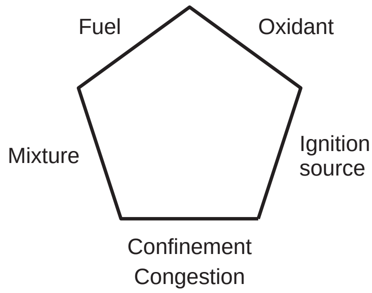

Figure 2: The explosion pentagon.

The fuel can be any finely divided solid material, capable of reacting rapidly and exothermically with a gaseous oxidizer (usually air). Characteristic particle sizes are in the range 1-100 μm. Flammable dust clouds can exist inside process equipment during normal operation, where high degree of confinement is inherently present. In a sufficiently confined and/or congested geometry, the release of chemical energy from the combustion process will result in a rapid increase in pressure, potential damage to structures, and possibly further escalation through structural collapse, outflow of material, impact of projectiles, etc. Dust flames represent a hazard to personnel, and may initiate fires.

The rate of combustion in dust clouds depends on parameters associated with the *fuel* (chemical composition, particle size distribution, etc.), the *oxidant* (chemical composition), the mixture (dust concentration, flow conditions, pressure, temperature, etc.), the *ignition source* (location, duration, total energy release, etc.), and the degree of *congestion* and *confinement* (i.e. geometrical boundary conditions). The strong effect of material properties on the reactivity of dust clouds implies that safety parameters, such as the maximum constant volume explosion pressure and rate of pressure rise, and hence the size-corrected maximum rate of pressure rise, better known as the K_{St} value, must be determined through testing of representative samples in standardized equipment. From a modelling point of view, this introduces a significant complication relative to gaseous fuels.

1.3.2 Historical perspective

The first scientifically investigated and documented dust explosion took place in the bakery of Mr Giacomelli in Turin on the evening of 14 December 1785 (di Bianzè, 1795; Eckhoff, 2003). It is likely that accidental dust explosions occurred in pre-industrial societies, but the hazard increased dramatically with the technological changes in agriculture, manufacturing, mining, transportation and storage that accompanied the industrial revolution (1750-1850). Dust explosion research in the 18th century focused on the role of coal dust in colliery explosions (Faraday & Lyell, 1845; Rice, 1911; Cybulski, 1975), and flour dust explosions in mills (Skjold & Eckhoff, 2012ab). Much of the early work on explosion protection focused on preventive measures, in particular the elimination of ignition sources (Price & Brown, 1922). One notable exception is the contribution by Hexamer (1883ab), who proposed the system illustrated in Figure 3 for explosion protection of malt mills. The concept combines explosion venting through pipes to the outside, explosion suppression by steam and explosion isolation by passive barriers (inherent safety). In modern terminology, the system included several layers of protection, and special features were included to account for the human factor.

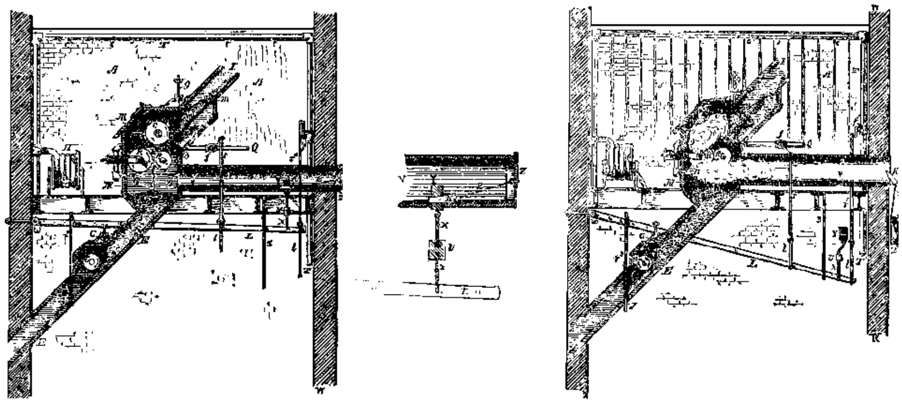

Figure 3: Vertical section of mill room with explosion protection system (Hexamer, 1883b)

The significant losses that occurred during World War II from exploding fuel tanks in combat airplanes motivated the development of modern systems for active explosion protection (Maisey, 1980). Graviner pioneered the development of systems applicable to industrial type of hazards (Grabowski, 1959; Moore, 1979; Maisey, 1980). Active explosion protection includes suppression and isolation.

Explosion venting is the most frequently used method of explosion protection. Venting is usually a passive measure, where destructive overpressures are prevented by designing parts of the enclosure to yield during early stages of the explosion, allowing combustion products and unburned dust to escape to the surroundings. The early guidelines for vent sizing were primarily of qualitative nature (Skjold *et al.*, 2008), but early large-scale investigations on the effect of vent size and ignition position on vented dust explosions demonstrated clearly that vent openings positioned close to the point of ignition provide the most effective pressure relief (Greenwald & Wheeler, 1925; Brown & Hanson, 1933).

The current practice of utilizing results from laboratory-scale dust explosion experiments in the design of explosion protection systems in industry originated in the 1950s (Hartmann, 1954; Hartmann & Nagy, 1957). Reliable test results require standardized equipment and procedures, and this resulted in the 1.2-litre Hartmann bomb (Dorsett *et al.*, 1960) and a similar 1.0-litre bomb in England (Raftery, 1968). The venting guidelines in Europe originate from the extensive amount of experimental work reported by Donat (1971) and Bartknecht (1971, 1974ab), and the theoretical analysis by Heinrich & Kowall (1971). Bartknecht (1971) introduced the *cube-root-law* and the standard 1-m^3 vessel. Eckhoff (1977) demonstrated the effect of turbulence on K_{St} values measured in the Hartmann bomb. Siwek (1977, 1988) introduced the 20-litre spherical bomb, and demonstrated good agreement with K_{St} values measured in the 1-m^3 vessel. However, Proust *et al.* (2007) presented results that show significant differences between K_{St} values obtained in the 20-litre sphere and the 1-m^3 vessel. Numerous researchers have studied the dispersion induced flow and transient combustion phenomena in 20-litre vessels: Pu (1988), Pu *et al.* (1988, 1990), Dahoe (2000), Dahoe *et al.* (1996, 2001abc), Skjold (2003), Pekalski (2004), Dyduch & Skjold (2010), Kalejaiye *et al.* (2010), Dahoe *et al.* (2013), etc.

1.3.3 The phenomenon

Dust explosions are inherently complex phenomena. A dust cloud is a mechanical suspension, i.e. a system of fine particles dispersed by agitation. Most dust samples have a relatively wide particle size distribution, and particles of different size react differently to variations in the flow field. This implies that the flow is inherently turbulent, the overall process is inherently transient, and the dynamics of the turbulent structures create local concentration gradients. Figure 4 illustrates some flow-related aspects of dust explosions. It is straightforward to classify the particle-laden flow in combustible dust clouds according to the particle volume fraction and relative particle spacing (Skjold, 2003; Skjold & Hansen; 2005). Dust concentrations ranging from the lower flammability limit (*LFL*), typically 20-60 g m^{-3}, to the most reactive mixtures, typically 500-750 g m^{-3}, are within the dilute suspension regime where two-way coupling should be accounted for (Elghobashi, 1994; Crowe *et al.*, 1998). As the dust concentrations approach the upper flammability limit, which could be in the range 2-10 kg m^{-3}, the flow enters the dense suspension regime where four-way coupling plays an important role.

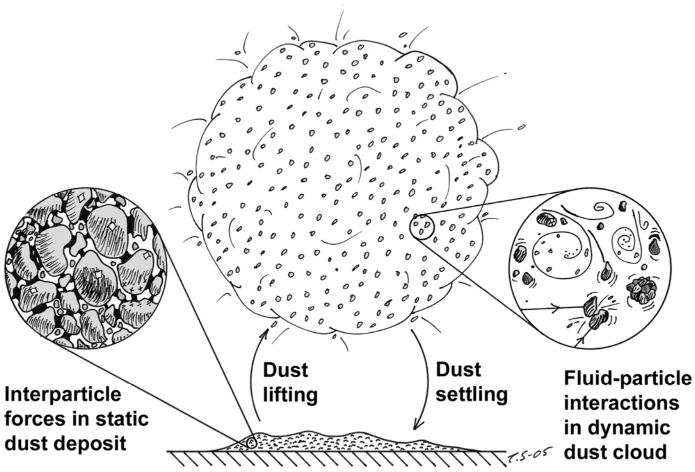

Figure 4: Dust clouds are mechanical suspensions (Skjold et al., 2006).

Flame propagation in dust clouds entails 'premixed combustion with non-premixed substructures' (Williams, 1986). Dust flames can be classified according to the combustion mechanisms for individual particles (Cassel, 1964; Bardon & Fletcher, 1983). Combustion in so-called *Nusselt flames* entails strictly heterogeneous reactions on the surface of the particles – this applies to materials such as carbon and refractory metals. The other category is *volatile flames*, where the particles produce vapour prior to gas-phase combustion (Rockwell & Rangwala, 2013) – the materials investigated in the present work (maize starch and coal dust) belong to this category. The structure of volatile flames varies significantly, depending on processes such as pyrolysis, evaporation, heat and mass transfer, chemical reactions, etc. (Gao *et al.*, 2013ab). For most organic solid materials, external heating of the fuel particles results in thermal degradation and liberation of volatiles through pyrolysis – the volatiles then burn in the surrounding atmosphere. This implies that the chemical species actually taking part in the combustion reactions may differ significantly from the overall composition of the fuel. Most combustible dust clouds encountered in industry are not monodisperse, and the particle size distribution has significant effect on the explosion violence (Eckhoff, 2003; Castellanos *et al.*, 2014).

The mechanism behind the flame acceleration process in dust explosions is the same as for gas explosions: expansion introduces flow, which generates turbulence, enhanced heat and mass transfer in the turbulent flow results in higher rate of combustion, which creates more expansion, which creates more turbulence, etc. (Bjerketvedt *et al.*, 1997). Dust explosions may escalate through the mechanisms of dust lifting ahead of the flame front and pressure piling in complex confined geometries.

1.3.4 The cube-root-law

The maximum explosion pressure P_{max} and the maximum rate of pressure rise $(dP/dt)_{max}$ for a dust sample are determined in standardized explosion vessels, such as the 20-litre vessel introduced by Siwek (1977, 1988). These parameters characterize the total energy release and the rate of reaction in dust explosions, respectively, and are used in the design of explosion protection systems. Scaling laws are required because $(dP/dt)_{max}$ depends on the volume V_v of the test vessel. The most frequently used scaling law is the *cube-root-law* (Bartknecht, 1971; Dahoe *et al.*, 1996, 2001b; Skjold, 2003):

$$K_{St} \equiv \left(\frac{dp}{dt}\right)_{\max} \left(V_v\right)^{1/3} = \text{constant} \tag{1}$$

Although it is practically impossible to realize the experimental conditions that fulfil the underlying assumptions behind the cube-root-law, the overall concept is valuable for practical applications. The so-called integral balance models seek to overcome some of the limitations with the cube-root-law (van der Wel, 1993; Dahoe *et al.*, 1996; Dahoe, 2000; Dahoe *et al.*, 2013).

The approach to scaling in the present work entails the use results obtained in standardized 20-litre explosion vessels as input to the combustion model in the CFD code DESC.

1.4 Computational fluid dynamics

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyse problems that involve fluid flow, with or without chemical reactions. Current use of CFD covers a broad range of applications, from fundamental theoretical studies involving models derived from first principles, to practical engineering calculations utilising phenomenological or empirical correlations.

Although the governing equations for turbulent fluid flow are well established (Bradshaw, 1994), analytical solutions are primarily of academic interest, and discrete solutions by direct numerical simulation (DNS) can only be realized for idealised systems. In recent years, models based on large eddy simulations (LES) have gained increasing popularity at universities. However, within the context of simulating industrial accident scenarios, most commercial CFD tools still rely on turbulence models based on the Reynolds-averaged Navier-Stokes (RANS) equations, such as the k-ε model (Launder & Spalding, 1974), complemented with sub-grid models that account for the influence of objects that cannot be resolved on the computational grid. For turbulent reactive flows, it is necessary to add models for chemical reactions, and to couple the resulting model system (Hjertager, 1981). When it comes to describing real industrial systems, it is important for users of advanced CFD tools to keep in mind that most simulations are inherently 'under-resolved', and that a significant degree of sub-grid modelling is required. This implies that solutions may not converge as the spatial or temporal resolution increases, and it is important to follow the grid guidelines provided by the software vendor.

1.4.1 FLACS

Many of the hazards encountered in society, and especially in the process industry, involve accident scenarios where fluid flow in large-scale complex geometries plays a key role (Skjold *et al.*, 2013b). FLACS is a specialised CFD tool developed especially to address process safety applications, such as release and dispersion of flammable, radioactive, asphyxiating or toxic material; gas, mist and dust explosions; propagation of blast and shock waves; and pool and jet fires (GexCon, 2014). The development of FLACS started at the Department of Science and Technology at Chr. Michelsen Institute (CMI) in 1980.

Numerical solver

The numerical solver in FLACS is a three-dimensional (3D) CFD code that solves Favre-averaged transport equations for mass, momentum, enthalpy, turbulent kinetic energy (k), rate of dissipation of turbulent kinetic energy (ε), mass-fraction of fuel and mixture-fraction on a structured Cartesian grid using a finite volume method (GexCon, 2014). The RANS equations are closed by invoking the ideal gas equation of state and the standard k-ε model for turbulence. FLACS solves for the velocity components on a staggered grid, and for scalar variables, such as density, pressure and temperature, on a cell-centred grid. The accuracy of the Flacs solver is second order in space and first/second order in time. FLACS uses the SIMPLE pressure correction scheme (Patankar, 1980), extended with source terms for the compression work in the enthalpy equation, for compressible flows, and the SIMPLEC scheme for non-compressible flows.

Combustion modelling

The purpose of a combustion model for premixed combustion is twofold: 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 default flame model in FLACS is the so-called β model (Arntzen, 1998), where flame thickness is constant, typically about three grid cells, and the flame propagates with a specified burning velocity defined by an empirical burning velocity model.

The empirical burning velocity model in FLACS originates from theory for flame stretch and experimental results for gaseous flames. The flame stretch of a flame surface element A_F is defined as:

$$\frac{1}{A_F}\frac{dA_F}{dt} \tag{2}$$

The Karlovitz stretch factor K for turbulent flames is defined as (Bradley, 1992):

$$K = \left(\frac{u'_{rms}}{\ell_\lambda}\right)\left(\frac{\delta_L}{S_L}\right) \tag{3}$$

where u'_{rms} is the root-mean-square of the turbulent velocity fluctuations, ℓ_λ is the Taylor scale, δ_L is the laminar flame thickness, and S_L is the laminar burning velocity. The Karlovitz stretch factor can be estimated by assuming that the laminar flame thickness is approximately equal to υ/S_L, where υ is the kinematic viscosity:

$$K \approx \frac{\nu\, u'_{rms}}{\ell_\lambda\, S_L^2} \tag{4}$$

In isotropic turbulence, K can be expressed as (Abdel-Gayed *et al.*, 1984):

$$K = \left[\frac{C_I}{15}\left(\frac{3}{2}\right)^{3/2}\right]^{1/2}\left(\frac{u'_{rms}}{S_L}\right)^2\left(\frac{\ell_I u'_{rms}}{\nu}\right)^{-1/2} = 0.1573\left(\frac{u'_{rms}}{S_L}\right)^2 \mathrm{Re}_e^{-0.5} \tag{5}$$

where ℓ_I is an integral length scale defined as $C_I k^{1.5}\varepsilon^{1}$, and C_I is equal to 0.202 (alternative expressions use the value 0.25 instead of 0.1573, and C_I =0.5).

Abdel-Gayed *et al.* (1987) used dimensionless parameters to correlate 1650 separate measurements of turbulent burning velocity for premixed gaseous mixtures. Bray (1990) expressed the data from Abdel-Gayed *et al.* by the empirical expression:

$$\frac{S_T}{S_L} = 0.875\, K^{-\varphi}\frac{u'_{rms}}{S_L} \tag{6}$$

Introducing the Karlovitz stretch factor leads to a general correlation for the turbulent burning velocity:

$$S_T = 0.875\left\{40.4^{-0.5}\left(\frac{u'_{rms}}{S_L}\right)^2\left(\frac{\ell_I u'_{rms}}{\nu}\right)^{-0.5}\right\}^{-\varphi}\frac{u'_{rms}}{S_L} \tag{7}$$

With the original value of the constant φ (0.392), this expression reduces to (Arntzen, 1998):

$$S_T = 1.81\cdot S_L^{0.784}\, u'^{\,0.412}_{rms}\, \ell_I^{0.196}\, \nu^{-0.196} \tag{8}$$

In FLACS, the kinematic viscosity υ is assumed to be constant and equal to 0.00002 $m^2\ s^{-1}$, and the correlation for turbulent burning becomes (Popat *et al.*, 1996):

$$S_T = 15.1\cdot S_L^{0.784}\, u'^{\,0.412}_{rms}\, \ell_I^{0.196} \tag{9}$$

Arntzen (1998) introduced the following modifications:

$$S_T = \min\begin{cases} S_{T1} = 8\, S_L^{0.284} u'^{0.912} l_m^{0.196} + S_L \\ S_{T2} = 15\, S_L^{0.784} u'^{0.412} l_m^{0.196} \\ S_{T3} = 110\, S_L^{4/3} l_m^{1/3} \end{cases} \tag{10}$$

where S_{T1} applies to low turbulence conditions, and S_{T1} accounts for quenching at high turbulence intensities. In practice, the burning velocity S_u relative to the unburnt mixture is calculated as:

$$S_u = \max \begin{cases} S_L \\ S_{QL} \\ S_T \end{cases} \quad (11)$$

where S_{QL} is the so-called quasi-laminar burning velocity (GexCon, 2014).

1.4.2 Dust explosion simulation code

Dust Explosion Simulation Code (DESC) was a project supported by the European Commission (EC), but DESC is also the name of the CFD code that represented one of the main deliverables from the DESC project (DESC, 2001).

Motivation

Current guidelines for explosion protection originate from experiments performed in relatively simple vessel arrangements, and are not necessarily applicable when dust explosions propagate through complex industrial plants. In principle, methods based on computational fluid dynamics (CFD) provide a more general approach to risk assessments, hence complementing existing standards and guidelines for process safety design, and thereby fulfilling essential health and safety requirements of ATEX 1999/92/EC (1999) in Europe.

The DESC project

The goal of the DESC project was to develop a CFD-based simulation tool for predicting the course of industrial dust explosions in complex geometries (Skjold, 2007). The European Commission supported the project through a cost-sharing contract under the Fifth Framework Programme (DESC, 2001). The participants in the consortium were Health and Safety Laboratory (HSL, project coordinator), GexCon AS, Nederlandse Organisatie voor toegepast-natuurwetenschappelijk onderzoek (TNO), Fraunhofer Institut für Chemische Technologie (Fraunhofer-ICT), INBUREX Consulting GmbH, Warsaw University of Technology (WUT), Technische Universiteit Delft (TU Delft), Forschungsgesellschaft für angewandte Systemsicherheit und Arbeitsmedizin (FSA), Øresund Safety Advisers AB, Hahn & Co and Lyckeby Culinar AB. Contributions were also received from Institut National de l'Environnement Industriel et des Risques (INERIS), Fike Europe Bvba and University of Bergen (UiB). GexCon developed the CFD code, and the other partners delivered experimental data and validation reports.

The DESC code

The CFD code DESC is a special version of FLACS. GexCon issued three *beta* versions DESC code prior to the release of DESC 1.0 in June 2006. Hansen *et al.* (2004) used the first *beta* version, DESC 1.0*b1*. Publications A to C used DESC 1.0*b2*, publications D used DESC 1.0*b3*, and publications F to M used DESC 1.0. The main difference between DESC 1.0*b2* and 1.0*b3* is a modification of the correlations used for the turbulent burning velocity. The primary feature added in DESC 1.0 was the possibility, at least in principle, of simulating explosion suppression systems.

Modelling of multiphase flow in DESC

The modelling of particle-laden flow and heterogeneous combustion in the CFD code DESC involves several simplifying assumptions (Skjold & Hansen, 2005; Skjold, 2007). The flow model assumes thermal and kinetic equilibria between the dispersed particles and the continuous phase (Marble, 1979), and the k-ε model in FLACS is unchanged for multiphase flows. This implies that current version of DESC cannot simulate phenomena such as agglomeration, gravitational settling, and selective separation of particles for flow through cyclones, bends or other curved paths. Future versions of DESC may utilize some of the more sophisticated models for particle-laden flows in FLACS (Ichard, 2012).

Combustion modelling in DESC

The combustion model used in DESC is essentially the same as in FLACS, including the β flame model (Arntzen, 1998) and the turbulent burning velocity correlation (Bray, 1990). Bradley, Chen & Swithenbank (1988) measured turbulent burning velocities in mechanical suspensions of maize starch particles dispersed in air, and found similar correlations between S_T/S_L, u'_{rms}/S_L and K as for gaseous fuel/air mixtures. This implies that the modelling approach in DESC applies to fine dusts of high volatile content, where flame propagation is driven principally by gas phase reactions. The thermodynamic data in FLACS, and the simple models for describing chemical equilibria in the combustion products (Arntzen, 1998), are limited to materials containing the elements carbon, hydrogen, oxygen, nitrogen and sulphur (CHONS). These simplifications limit the application area of DESC to certain classes of materials, and flame propagation in dust clouds with relatively high reactivity. The experience thus far suggests that the model works best for organic materials with K_{St} values of at least 100 bar m s^{-1}, and preferably higher. Both the maize starch dust and the coal dust investigated in this thesis have K_{St} values of about 150 bar m s^{-1}.

Modelling of turbulent flame propagation according to Eq. (9) requires estimates for the laminar burning velocity S_L as function of dust concentration. The approach adopted for the first versions of DESC was to extract combustion parameters from pressure-time histories measured in standardized 20-litre explosion vessels (ASTM E 1226, 2000; EN 14034-1, 2004; EN 14034-2, 2006). This approach has the several advantages: there are numerous 20-litre explosion vessels in operation worldwide, testing of one dust sample takes about 1-2 days, and the influence of numerous parameters, including chemical composition and particle size distribution, is lumped into one parameter. Figure 5 shows typical pressure-time curves obtained from dust explosion tests in a 20-litre explosion vessel – the black curve is obtained in a test ignited with a 6 J electric arc, and the red curve illustrates the effect of using two 5 kJ chemical igniters on the pressure development.

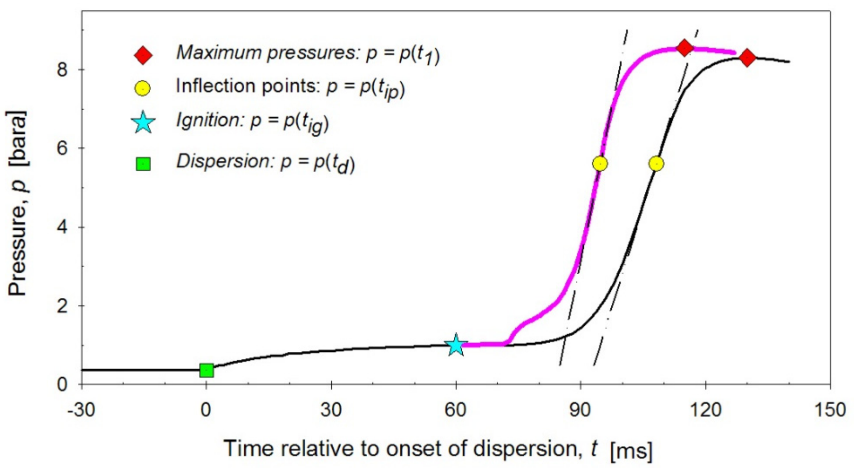

Figure 5: Typical pressure-time curves from a 20-litre explosion vessel (Skjold et al., 2006b).

To avoid the complications introduced by energetic ignition sources, and to minimize wall effects, the analysis focuses on values estimated in the inflection point of the pressure-time curves (at time t_{ip}). Assuming Eq. (9) to be valid for flame propagation in dust clouds, an inverse version of Eq. (9) provides an estimate for the laminar burning velocity, for a given dust concentration:

$$\tilde{S}_L\left(t_{ip}\right) = C_L\, 0.0315\left[S_T\left(t_{ip}\right)\right]^{1.276}\left[u'_{rms}\left(t_{ip}\right)\right]^{-0.526}\left[\ell_I\left(t_{ip}\right)\right]^{-0.250} \quad (12)$$

where the non-dimensional constant C_L is introduced to account for uncertainties in the assumptions behind the estimates for S_T, u'_{rms} and ℓ_I.

The estimate for turbulent burning velocity follows from the thin flame approximation for the turbulent burning velocity in a spherical vessel yields (Dahoe *et al.*, 1996):

$$S_T(t_{ip}) = \frac{1}{3(p_f - p_i)} \underbrace{\left(\frac{dp}{dt}\right)_m V_v^{1/3}}_{K_{St}} \left(\frac{3}{4\pi}\right)^{1/3} \left(\frac{p(t_{ip})}{p_i}\right)^{-1/\gamma} \left\{1 - \left(\frac{p_f - p(t_{ip})}{p_f - p_i}\right)\left(\frac{p(t_{ip})}{p_i}\right)^{-1/\gamma}\right\}^{-2/3} \tag{13}$$

where p_i and p_f are the initial and final absolute pressures, respectively, γ is the specific heats ratio (assumed equal to 1.40), and V_v is the volume of the explosion vessel. It is likely that more sophisticated models, that take into account the thickness of the flame, will replace Eq. (15) in the future (Dyduch & Skjold, 2010; Dahoe *et al.*, 2013).

The estimates for u'_{rms} and ℓ_I in the inflection point of the pressure time curve rely on empirical decay laws reported by Dahoe (2000) and Dahoe *et al.* (2001a). The estimate for turbulence intensity is:

$$u'_{rms}(t_{ip}) = u'_{rms}(t_0)\left(\frac{t_{ip}}{t_0}\right)^n \tag{14}$$

with u'_{rms} (t_{ip}), t_0 and n equal to 3.75 m s^{-1}, 0.060 s and -1.61, respectively. The corresponding expression the turbulent integral length scale is:

$$\ell_I(t_{ip}) = \ell_I(t_0)\exp\left(a_1 \ln\left(\frac{t_{ip}}{t_0}\right) + a_2\left\{\ln\left(\frac{t_{ip}}{t_0}\right)\right\}^2\right) \tag{15}$$

where a_1, a_2, $\ell_I(t_{ip})$ and t_0 are –3.542, 1.321, 0.012845 m, and 0.0588 s, respectively. Equations (14) and (15) and used in the range 0.060 s < t < 0.200 s, relative to onset of dust dispersion.

Since chemical reactions in dust-air mixtures seldom go to completion (Lee, 1988), the combustion model in DESC requires an estimate of the mass fraction of fuel λ that is converted to combustion products. 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 the specific heats and heats of formation of reactants and products, and the ratio between gaseous species in reactants and products.

In the CFD simulations, Eq. (9) defines the turbulent burning, the k-ε turbulence model provides an estimate for u'_{rms}, and ℓ_I is estimated from the algebraic expression:

$$\tilde{\ell}_I = \min\begin{cases} 0.025\, R_F \\ 0.08\, L_S \end{cases} \tag{16}$$

where R_F is the flame radius and L_S is the minimum spatial dimension of solid boundaries surrounding the flame. The modelling in DESC 1.0 does not include the expressions for S_{T1} and S_{T3} in Eq. (10), nor the expression for the quasi-laminar burning velocity S_{QL} in Eq. (11).

Discusssion

The results presented in the Publications show that the general results obtained with DESC 1.0 for various dust explosions scenarios with maize starch and coal dust are reasonably good, given the complexity of the physical and chemical phenomena involved, and the simplicity of the model system. However, the model predictions vary significantly with grid resolution, and the 'optimal' value for the non-dimensional constant C_L vary from 0.75 for the 0.03 m cubical grid cells used in Publication M to 1.25 for some of the larger geometries. For some of the experiments there is obviously significant uncertainty associated with the reactivity of the dust.

Some results indicate that the correlation between S_T and u'_{rms} should be more linear than the exponent (0.412) for u'_{rms} in Eq. (9) predicts (Skjold, 2007). Simulation results for a series of large-scale gas explosion experiments in unconfined congested geometries (Evans *et al.*, 1999) indicate the same for FLACS. Further efforts to improve and validate the models system will entail the implementation of an integrated framework for validation and testing (Skjold *et al.*, 2010b).

1.5 Experimnets

This paragraph introduces the equipment used in the experiments, and provides reference to experimental procedures and results. Given the close relation between the modelling of turbulent combustion in FLACS and DESC, the experiments aim at exploring flame propagation in premixed gaseous mixtures and mechanical suspensions of dust dispersed in air under similar flow conditions.

1.5.1 The 20-litre USBM vessels

Figure 6 illustrates the 20-litre USBM vessel at the Department of Physics and Technology, University of Bergen. Skjold (2003) describes the equipment in more detail, including experimental procedures and the spark/arc generator. Publications A-K use experimental results from this vessel in the empirical combustion models for the various dusts.

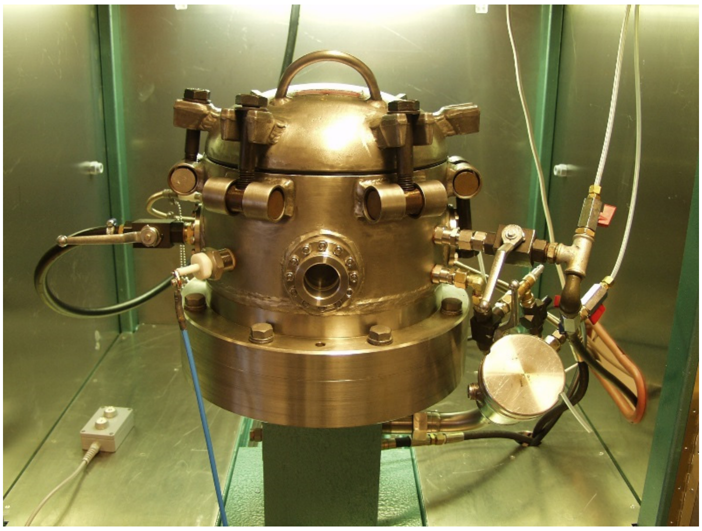

Figure 6: The 20-litre USBM vessel at the Dust Explosion Laboratory at UiB.

1.5.2 The balloon experimnet

Figure 7 shows the original drawing for the dispersion nozzle and spark gap for the second generation of the balloon experiment for dust clouds. Publication L describes experimental procedures and presents results.

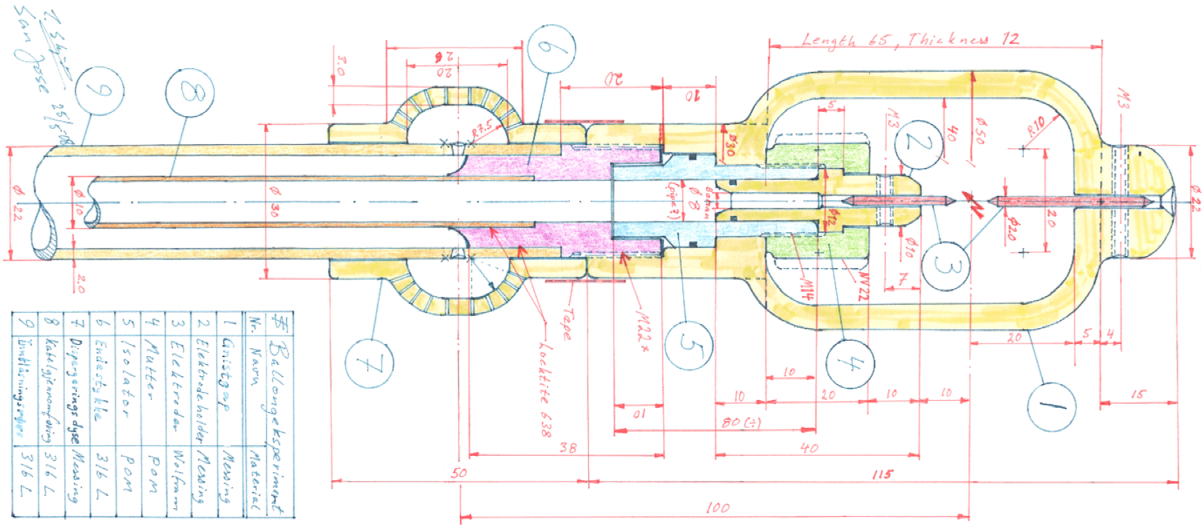

Figure 7: Spark gap and dispersion nozzle in the latest version of the balloon experiment.

1.5.3 The 3.6-m flame acceleration tube

Figure 8 shows the technical drawings for the 3.6-m flame acceleration tube. Publication M describes the experimental procedures and presents results from the experiments.

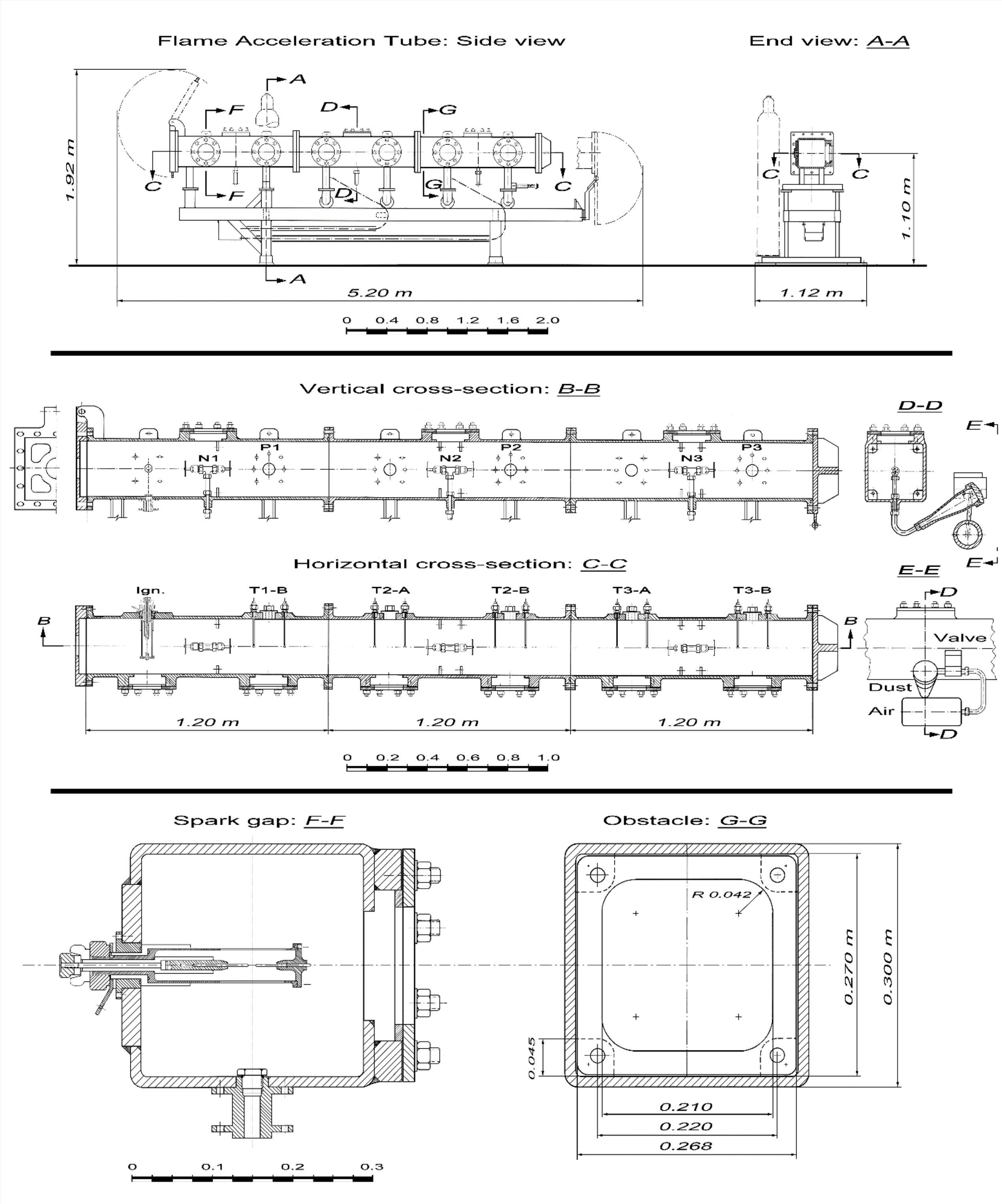

Figure 8: Technical drawing of the 3.6-m flame acceleration tube.

2. Summary of publications

This chapter summarizes the content of the 13 publications and describes the relation between them. Publications A-K describe the development and validation of the CFD code DESC, from the beta versions 1.0b2 (publications A-C) and 1.0b3 (Publication D), to the first official version (1.0) that was released in June 2006 (publications E-K). The two last publications describe experimental studies of flame propagation, one in transparent balloons (Publication L), and the other in a 3.6 m flame acceleration tube (Publication M). Publication M includes comparison between experimental results and CFD simulations with FLACS 10.2 and DESC 1.0.

2.1 Publication A

The paper *"Simulating dust explosions with the first version of DESC"* (Skjold *et al.*, 2005a) is an updated version of a paper presented at HAZARDS XVIII in Manchester, 23-25 November 2004 (Skjold *et al.*, 2004a). The work on this paper progressed in parallel with publications B and C, and all three papers describe the modelling in DESC 1.0b2. In this context it should be mentioned that several earlier publications from GexCon describe the possibility of using FLACS for simulating dust explosions (van Wingerden, 1996; van Wingerden *et al.*, 2001; Arntzen *et al.*, 2003; Siwek *et al.*, 2004), and that various conference papers describe earlier prototypes of DESC (Hansen *et al.*, 2004; Skjold & Hansen, 2005; Hansen *et al.*, 2005). However, publications A and B were the first journal publications to document the modelling concept adopted for DESC. Both papers describe the use of pressure-time histories measured in standardized 20-litre laboratory tests for estimating the laminar burning velocity S_L and the fraction λ of the available fuel that reacts, and the subsequent use of these results as input to the combustion model in DESC 1.0b2.

Publication A describes laboratory-scale experiments with maize starch and the procedure for generating an empirical combustion model in DESC 1.0b2. Note that there is an error in the system of correlations for the turbulent burning velocity: Eq. (3) should be identical to Eq. (3) in Publication B. The main differences between the modelling in DESC 1.0b2 (papers A-C), and the modelling in the later versions (papers D-K and M) are:

- In DESC 1.0b2, the estimates for the laminar burning velocity assumed a constant integral length scale of 0.006 m in the 20-litre vessel, based on simulations with FLACS (Skjold, 2003). The modelling in DESC 1.0b3 and 1.0 assumes that the integral length scale in the 20-litre vessel follows the empirical expression reported by Dahoe (2000) and Dahoe *et al.* (2001c).
- In DESC 1.0b2, the value for the burnable fuel fraction λ was set to zero at the lower flammability limit (see figures 2, 5 and 4 in publications A, B and C, respectively). In the later versions, the value of λ at the lower flammability limit is estimated by extrapolating values determined at higher nominal dust concentrations (see Fig. 4 in Publication D).
- The system of three correlations for the turbulent burning velocity S_T used in DESC 1.0b2 (Eq. 3 in Publication B) is reduced to one single correlation in DESC 1.0b3 and 1.0 (Eq. 4 in Paper D). This modification represented a significant simplification of the analysis of the results from the 20-litre vessel, without any apparent loss of accuracy in the model system.

Publication A demonstrated the performance of DESC 1.0b2 for two test cases: vented dust explosions with maize starch in a 9.4 m^3 silo (Hauert *et al.*, 1996), and constant volume dust explosions with coal dust and toner in a system consisting of two vessels connected by a pipe (Lunn *et al.*, 1996). The simulations over-predict the reduced explosion pressures for the silo explosions, but reproduce the experimental trends well. The results obtained for the interconnected vessel system were in reasonable agreement with experimental values obtained for different ignition positions, indicating that the model system can simulate the effect of pressure-piling. The empirical combustion model used in the simulations relied on experimental data obtained for maize starch of type Meritena A, from the same batch that was used in the experiments simulated in Publication B (Eckhoff *et al.*, 1985; 1987), and not samples from the dusts that were actually used in the experiments simulated in Publication A. This represents a significant source of uncertainty in the results. The grid resolutions in the simulations were 0.10 and 0.08 m for the vented silo and connected vessel system, respectively, and the estimates for the laminar burning velocity were not adjusted (i.e. $C_L = 1.00$).

Publication A elaborated on the possibility of implementing alternative correlations for turbulent flame propagation in future versions of DESC, with particular focus on the system of equations proposed by Dahoe (2000) and Dahoe *et al.* (2001c). Some work has been done in this area, particularly with respect to using more elaborate methods for extracting combustion parameters from measured pressure-time histories in 20-litre vessels (Skjold *et al.*, 2008; Dyduch & Skjold, 2010; Dahoe *et al.*, 2013). In order to estimate burning velocities and flame thicknesses from pressure-time data, it is desirable to use a relatively weak ignition source. However, the poor repeatability of dust explosion experiments in the 20-litre vessel, when ignited with a weak ignition source, represents a significant source of uncertainty in the analysis (Skjold, 2003; Dyduch & Skjold, 2010). Results presented in Publication L suggest that the initial phase of flame propagation in a turbulent dust cloud can be significantly influenced by partial quenching and distributed combustion. It is nevertheless likely that the modelling of flame propagation in future versions of DESC will entail the use of separate correlations for turbulent burning velocity and turbulent flame thickness.

2.2 Publication B

The paper *"Simulation of dust explosions in complex geometries with experimental input from standardized* tests" (Skjold *et al.*, 2006a) is an updated version of a paper presented at the Fifth International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions (ISHPMIE) in Krakow, 10-14 October 2004 (Skjold *et al.*, 2004b). This paper describes the modelling in DESC 1.0b2 (see the description of Publication A for details).

Publication B demonstrated the methodology for estimating laminar burning velocities from pressure-time histories measured in 20-litre explosion vessels. The procedure was first applied to data for turbulent propane-air mixtures ignited to deflagration in the standard 20-litre USBM vessel (Skjold, 2003). Given the simplicity of the method, the estimates compare reasonably well with values from literature. Following the same procedure for maize starch results in the empirical model used for simulating a series of dust explosion experiments performed in a vented 236-m^3 silo (Eckhoff *et al.*, 1985; 1987). The results show that DESC 1.0b2 predicts explosion pressures in reasonable agreement with the experiments, with a tendency towards over-prediction for ignition in the central part of the silo. The simulations used a relatively coarse grid, 0.50 m cubical grid cells, and the laminar burning velocity was enhanced by 10 % ($C_L = 1.10$). Publication J revisits the experiment in the 236-m^3 silo, and includes simulations with two different grid resolutions: 0.176 and 0.263 m cubical grid cells.

2.3 Publication C

The paper *"Simulating the influence of obstacles on accelerating dust and gas flames"* (Skjold *et al.*, 2005b) was presented as a poster at Twentieth International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS) in Montreal, 31 July - 5 August 2005. This paper describes validation of the models in DESC 1.0b2 (see the description of Publication A for details).

Publication C explored flame acceleration by repeated obstacles and the effect of grid resolution on the simulation results. The experiments reported by Pu (1988) and Pu *et al.* (1988a) entail flame propagation in methane-air mixtures and mechanical suspensions of maize starch in air, under similar initial flow conditions, in a closed tube with diameter 0.19 m and length 1.86 m. Simulation results obtained with FLACS for the methane-air mixtures were in good agreement with experimental results, but the simulations with DESC of tests with maize starch significantly over-predicted the observed flame speeds. It should be noted that the finest grid resolutions used in these simulations (9.5 and 19 mm) are not consistent with current grid guidelines for FLACS and DESC, and that the laminar burning velocities estimated from the 20-litre vessel was not adjusted (i.e. C_L = 1.00).

Publication C was important for the development of DESC. The results clearly demonstrated the strong influence of grid resolution on simulation results obtained with FLACS and DESC. The spatial scale of the experiment made it necessary to take into account the effect of radiative heat losses during flame propagation. The work by Pu and co-workers was the primary inspiration for the construction of the flame acceleration tube described in Publication M.

2.4 Publication D

The paper *"Possibilities, limitations, and the way ahead for dust explosion modelling"* (Skjold *et al.*, 2006b) was presented at HAZARDS XIX in Manchester, 28-30 March 2006. This paper describes the modelling in DESC 1.0b3, which is essentially identical to the modelling in DESC 1.0.

Publication D summarizes the modelling in DESC 1.0b3, and demonstrates how a CFD code for dust explosions can be used to optimize the design of a vent duct installed on a drier. The example was taken from a consulting project, and reproduced with permission from the costumer. The paper concludes with some thoughts about the way ahead for dust explosion modelling, in light of current knowledge about dust explosions and inherent limitations with respect to modelling capabilities.

2.5 Publication E

The paper *"Modelling of vented dust explosions – empirical foundation and prospects for future validation of CFD codes"* (Skjold *et al.*, 2008) was presented at HAZARDS XX in Manchester, 23-25 November 2008. The modelling in DESC 1.0 is essentially identical to the modelling in DESC 1.0b3, with the notable exception that DESC 1.0 includes a transport equation for a second mixture fraction. The second mixture fraction is required when simulating the effect of inert atmospheres and suppression agents on flame propagation (van Wingerden & Skjold, 2008; van Wingerden *et al.*, 2009), and does not influence the work presented here.

Publication E reviews the development of venting guidelines for dust explosions, and presents simulation results obtained with DESC for a series of dust explosion experiments in a 64 m^3 vented enclosure (Tamanini & Chaffee, 1989; Tamanini, 1990). These experiments were particularly relevant when the paper was written, since the results describe the effect of the initial level of turbulence on the reduced explosion pressure in vented dust explosions. This information was incorporated in the 2007 edition of the NFPA 68 guideline (NFPA 68, 2007; Zalosh, 2007). The maize starch dust used in the experiments in the 64 m^3 enclosure was significantly more reactive than the dust used to define the empirical combustion model, and the laminar burning velocities estimated from the 20-litre vessel were therefore increased by 75 % (i.e. C_L = 1.75). The simulation results show that DESC reproduces the decay of turbulence following the dust dispersion process quite well, and the simulated explosion pressures are in reasonable agreement with the trends observed in the experiments. However, the simulation results vary significantly between the two grid resolutions, 0.10 and 0.20 m cubical grid cells, and this uncertainty represents an inherent limitation with respect to the applicability of the CFD code for industrial safety.

2.6 Publication F

The paper *"Simplified modelling of explosion propagation by dust lifting in coal mines"* (Skjold *et al.*, 2007) was presented at the *Fifth International Seminar on Fire and Explosion Hazards* (ISFEH) in Edinburgh, 23-27 April 2007.

Publication F describes the modelling of dust lifting from a layer in DESC. The empirical model for dust lifting originates from experimental work at Warsaw University of Technology (Klemens *et al.*, 2006; Zydak & Klemens, 2007). The first part of the paper presents results from simulations of the original laboratory-scale experiments. The simulations represent the experimental trends fairly well, but the results vary significantly with grid resolution and the distribution of porosities in the grid cells close to the solid surface. The second part of the paper demonstrates the performance of the model system by simulating large-scale dust explosion experiments conducted in a 100-m surface gallery at the Experimental Mine Barbara in Katowice (Lebecki *et al.*, 1993; Wolanski, 1993; Lebecki *et al.*, 1995). The simulated scenarios include sensitivity studies with respect to the value of an empirical constant in the model for dust lifting, for three different burning velocities (C_L: 0.75, 1.00 and 1.25). In the experiments, the chain of events started with a methane explosion and continued with a dust explosion fuelled by dust lifting from the layers. This could not be simulated with FLACS/DESC, since the code does not allow for the use of two different fuels in the same simulation (the second mixture fraction only works for inert components). The premixed methane-air cloud was therefore replaced with a dust cloud in the simulations. The results demonstrate that the dust lifting model can produce reasonable results, even when applied to large-scale explosion scenarios.

2.7 Publication G

The paper *"Simulating the effect of release of pressure and dust lifting on coal dust explosions"* (Skjold, 2007b) was presented at the Twenty-first International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS) in Poitiers, 23-27 July 2007.

Publication G describes simulations where DESC 1.0, including the dust lifting model described in Publication F, was used to simulate a classical series of experiments with coal dust in a 229 m long, 2.3 m diameter, surface gallery (Greenwald & Wheeler, 1925). Publication H describes the empirical model for the coal dust. The results are quite sensitive with respect to the reactivity of the coal dust (C_L: 1.00, 1.25, 1.50, 1.75 and 2.00), and there is significant uncertainty associated with both the quality of the measurements and the actual reactivity of the coal dust. The simulations nevertheless indicate that CFD simulations with a simple empirical model for dust lifting can produce reasonable results when applied to large-scale accident scenarios.

2.8 Publication H

The paper *"Review of the DESC project"* (Skjold, 2007a) is an updated version of a paper presented as the opening plenary lecture at the Sixth International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosions (ISHPMIE) at Dalhousie University in Halifax, 27 August 27 - 1 September 2006 (Skjold, 2006).

Publication H summarizes the main results from the seven work packages in the DESC project, with particular focus on aspects related to the modelling of flow and combustion in the CFD code DESC 1.0. The paper elaborates on the methodology for estimating laminar burning velocities from pressure-time histories measured in 20-litre explosion vessels. The results indicate a near linear dependence on the root-mean-square of the turbulent velocity fluctuations for the turbulent burning velocity (Fig. 3), which is consistent with results presented by Tai *et al.* (1988).

The paper presented results from a DESC simulation of a coal dust explosions in an interconnected vented vessel system, consisting of a 20 m^3 primary vessel and a 2 m^3 secondary vessel connected by a 0.50 m diameter pipe with a 90^o bend. HSL performed a series of experiments in this vessel system as part of the DESC project (Holbrow, 2004; Holbrow 2005ab), and DESC over-predicts the explosion pressure in the secondary vessel for most of these tests. There notable exception is test no. 13 with coal dust, which produced an overpressure of about 0.5 bar in the primary vessel, and close to 3 bar in the secondary vessel. The DESC simulation of test no. 13 presented in Publication H predicts the pressure in the primary vessel reasonably well, but the simulated pressure in the secondary vessel is only about 2 bar. Publication I revisits test no. 13 in the interconnected vented vessel system.

2.9 Publication I

The paper *"Flame propagation in dust clouds: challenges for model validation"* (Skjold, 2010a) was presented at the *Eighth International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions* (ISHPMIE) in Yokohama, 5-10 September 2010.

Publication I revisits some of the experiments with coal dust in the interconnected vented vessel system (Holbrow, 2004; Holbrow 2005ab), and in particular test no. 13 described in Publication H. The paper describes a sensitivity analysis with respect ignition delay time, ignition position and grid resolution for test no. 13, as well as the effect of reactivity for tests 13, 33 and 34 – i.e. for different ignition positions in the primary vessel.

For test no. 13, the results reveal that the simulated maximum explosion pressure in the secondary vessel is very sensitive to modest changes in ignition position. Moving the point of ignition 0.6 m towards the rear wall results in almost identical explosion pressures as observed in the experiment. Moving the point of ignition 0.6 m towards the vent opening reduces the pressure to less than half the experimental value. The highest pressure occurs when the flow through the connecting pipe disperses the dust layer in the pipe just in time for the resulting dust cloud to fill the secondary vessel with flammable mixture immediately before the flame arrives. Small changes in the ignition position alters the dynamics of the dust lifting and flame propagation process, and air from the pipe dilutes the mixture in the secondary vessel before the flame arrives.

The general results for the three tests show that the maximum explosion pressures predicted by DESC are sensitive to the reactivity of the mixture (C_L = 1.00, 1.25 and 1.50), and that DESC generally over-predicts the explosion pressure in the secondary vessel. A likely explanation for this can be that various phenomena that are not modelled in DESC may contribute to lower explosions pressures in the experiments: turbulent quenching and distributed flame propagation during the initial phase of flame propagation (see Publication L), fall-out of dust, etc.

Publication I concludes with a discussion of knowledge gaps, including the need for repeated large-scale explosion experiments for model validation. It is a paradox that very few experimental studies of explosion phenomena at large spatial scales include repeated tests, whereas the ones that actually include repeated tests often show large scatter in the results, even for premixed mixtures of gaseous fuel in air (e.g. Evans *et al.*, 1999).

2.10 Publication J

The paper *"Simulating vented maize starch explosions in a 236 m^3 silo"* (Skjold, 2014) was presented at the Eleventh International Symposium on Fire Safety Science at University of Canterbury, 10-14 February 2014.

Paper J revisits the large-scale dust explosion experiments performed in a vented 236-m^3 silo at Stordalen (Eckhoff *et al.*, 1985; 1987). Publication B described simulations of the same experiments with DESC 1.0b2, on a relatively coarse grid (0.5 m cubical grid cells and C_L = 1.10). The simulations with DESC 1.0 in Publication J used smaller grid cells and included the effect of grid resolution (0.176 and 0.263 m cubical grid cells; C_L = 1.00). The simulated maximum explosion pressures are generally higher than the corresponding experimental values, especially for ignition in the central part of the silo. Partial quenching and convective transport of the initial flame kernel by the particle-laden jets exiting about 5.5 m above the silo bottom from a vertical pipe may explain the over-prediction observed for explosions ignited near the centre of the silo. Such effects are not modelled in DESC, but may occur in practice (see Publication L). The effect of grid resolution is most pronounced for the lowest explosions pressures, with ignition in the upper part of the silo.

2.11 Publication K

The paper *"Validation of the DESC code in simulating the effect of vent ducts in dust explosions"* (Castellanos *et al.*, 2013) is a modified version of a paper presented at Twenty-third International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS) in Irvine, 24-29 July 2011 (Castellanos *et al.*, 2011a).

Publication K reviews experimental work on the effect of vent ducts on the maximum reduced explosion pressure in coal dust explosions, and compares predictions from various venting guidelines and simulations with DESC 1.0 to experimental results reported by Lunn *et al.* (1988) and Hey (1991). The simulations used the same empirical combustion model for coal dust as publications H and I, with C_L = 1.25 in most of the simulations (based on the sensitivity analysis reported in Publication I). The results from the simulations are generally in good agreement with the experiments. The reduced maximum overpressures increase systematically with increasing duct length, and closed-end ignition represents the worst-case scenario. The significant spread in the experimental results for repeated tests poses a challenge for the validation of DESC, and also for the development of empirical correlations.

2.12 Publication L

The paper *"A constant pressure dust explosion experiment"* (Skjold *et al.*, 2013a) is a modified version of a paper presented at the Fourteenth Annual Symposium of the Mary Kay O'Connor Process Safety Center at College Station, 25-27 October 2011 (Skjold *et al.*, 2011). Skjold & Eckhoff (2006) and Skjold *et al.* (2008a) presented results from earlier versions of the balloon experiment.

Publication L describes explosion experiments in transparent latex balloons. The idea behind this study was to explore the use of a constant pressure experiment for dust explosion, to complement the experiments in constant volume explosion vessels, and to compare flame propagation in different fuel-air mixtures under similar initial conditions. The flammable mixtures investigated include:

- Initially quiescent propane-air mixtures, ignited by spark discharges
- Initially turbulent propane-air mixtures, ignited by spark discharges 1 s after onset of air injection
- Mechanical suspensions of either spores of *Lycopódium clavátum* or maize starch (Meritena A), ignited by 40 J chemical igniters 1 s after onset of dust dispersion

The results obtained for initially quiescent propane-air mixtures illustrate the concept of determining flame speeds and burning velocities from measurements of the increase in flame radius with time, for mixtures with known expansion ratio (Strehlow & Stuart, 1953). Unfortunately, it was not straightforward to determine unambiguous values for the flame radius in dust clouds. At relatively low dust concentrations, the flames propagated in a distributed manner and eventually died out. At higher concentrations, the flames could still propagate in a distributed manner initially, but after reaching a certain critical size the mode of flame propagation resembled that of gaseous flames. Still, it was not straightforward to determine an unambiguous flame front for the dust flames, due to diffraction when the radiation from the flame passes through the unreacted dust cloud.

The distributed mode of flame propagation in dust clouds under turbulent flow conditions, accompanied by limited energy release, may explain the seemingly random delay in the pressure rise observed in constant volume dust explosion experiments with weak ignition sources (Skjold, 2003; Skjold *et al.*, 2010), and possibly also the large spread in results, and the relatively low maximum explosion pressures, for tests with bottom injection and ignition 7.5 m above the silo bottom (i.e. tests 14, 15, 16, 18 and 19) in the explosion experiments reported by Eckhoff *et al.* (1985, 1987).

2.13 Publication M

The paper *"Experimental and numerical investigations of constant volume dust and gas explosions in a 3.6-m flame acceleration tube"* (Skjold *et al.*, 2014) is an upgraded version of a paper presented at the Ninth International Symposium on Hazard, Prevention and Mitigation of Industrial Explosions (ISHPMIE) in Krakow, 22-27 July 2012 (Skjold *et al.*, 2012a). The development of the 3.6-m flame acceleration tube started in the autumn of 2004. Several publications have reported preliminary and/or complementing results (Skjold *et al.*, 2009; Enstad, 2009; Kalvatn, 2009; Skjold, 2010b; Skjold & Castellanos, 2011ab; Olsen, 2012).

Publication M describes an experimental investigation of turbulent flame propagation in propane-air mixtures, and in mechanical suspensions of maize starch dispersed in air. The flame acceleration tube is a closed vessel of length 3.6 m and internal cross-section 0.27 m × 0.27 m, equipped with systems for dust dispersion, ignition, pressure and flame measurements, and data acquisition.

The primary motivation for the work was to gain improved understanding of turbulent flame propagation in dust clouds, with a view to develop improved models and methods for assessing explosion risks in the process industry. Selected experiments were simulated with the computational fluid dynamics codes FLACS and DESC. The results obtained from experiments with initially turbulent propane-air mixtures were in good agreement with CFD simulations with FLACS for concentrations up to about 6 vol.% propane in air. For higher fuel concentrations the simulations under-predict the explosion violence. Flame propagation in the propane-air mixtures was significantly influenced by the initial flow conditions, and less sensitive to the nature of the ignition source.

The results obtained for mechanical suspensions of maize starch dispersed in air varied significantly for the same experimental conditions. It was nevertheless possible to identify a subset of experiments that showed good repeatability, and these results were in reasonable agreement with CFD simulations with DESC. Although the overall results from the CFD simulations are in reasonable agreement with the experimental results, there is significant potential for improving the numerical models.

3. Conclusions and suggestions for further work

This dissertation consists of 13 publications that describe the development and validation of a methodology for estimating the consequences of accidental dust explosions in complex geometries. The approach adopted entails the use of results from tests in standardized 20-litre explosion vessels as input to the combustion model in the CFD code DESC, and the subsequent validation of the model system by comparing results from large-scale experiments with predictions from CFD simulations. In addition to dust explosion experiments in 20-litre vessels, the PhD project includes dedicated laboratory experiments designed to explore selected aspects of flame propagation in dust clouds. Since DESC is a special version of the CFD code FLACS for gas explosions, it is particularly interesting to compare flame propagation in gaseous mixtures and mechanical suspensions of combustible powder in air under similar experimental conditions.

3.1 Conclusions

The overall conclusions from the work described in this dissertation are:

1. The development, validation and use of the CFD code DESC indicate that numerical modelling of dust explosions can represent a valuable addition to existing methods for consequence assessments and design optimization in the process industry.
2. Although the overall results from the CFD simulations are in reasonable agreement with the experimental results, there is significant potential for improving the numerical models further.
3. Both experiments and CFD simulations show that the course of dust explosions in complex geometries may change dramatically for moderate variations in the initial and boundary conditions. These observations emphasize the need for repeated large-scale experiments, and should have implications for the way scientists and engineers derive, communicate and use empirical correlations for the design of explosion protection systems.
4. The simulation results obtained with DESC and FLACS vary significantly with changes in grid resolution. The results from the validation work show that tuning the reactivity of the mixture to some extent compensates for this effect. This implies that reliable simulation results requires strict adherence to grid guidelines.
5. The significant effect of radiative heat losses on flame propagation in elongated vessels at laboratory scale complicates the analysis of the experimental results. It is not straightforward to isolate the effect of heat losses to the wall from that of a thickened reaction zone or volumetric combustion behind the flame zone.

3.2 Suggestions for further work

Future efforts towards improved modelling of flame propagation in dust clouds should focus on the following topics:

a) There is an urgent need to implement a new numerical solver in FLACS and DESC that supports local grid refinement. This is necessary to limit the influence of grid resolution on the simulation results, and for resolving complex internal geometries in DESC.

b) Given that the primary application area for the CFD codes FLACS and DESC is industrial safety, any significant modifications to the combustion models will require extensive validation. To this end, it is essential to establish an integrated framework for model validation. The validation framework should support the documentation of capabilities and inherent limitations of the model system, automated verification and testing (Skjold *et al.*, 2013), sensitivity studies and parameter optimization (Pedersen *et al.*, 2013), and eventually reliable estimation of confidence intervals for model predictions (McGrattan *et al.*, 2014).

c) The modelling of turbulent particle-laden flows may be improved, including particle-turbulence interactions, settling effects, etc. (Ichard, 2012). The main challenge will be to limit the computational cost associated with more sophisticated model concepts.

d) There is also significant potential for improving the modelling of flame propagation in dust clouds, including the production of volatile components (Rockwell & Rangwala, 2013), quenching effects, distributed combustion, flame thickness (Dahoe *et al.*, 2013), heat transfer by radiation, etc.

There is also a need for further work on the experimental side:

e) Future experimental studies should explore alternative measurement techniques for flame detection, such as optical probes or ionization gauges.

f) Future research on dust explosion can benefit significantly from standardization and sharing of technology that supports reliable and affordable measurements of parameters such as dust concentration, turbulence intensity, flame temperature, radiative heat transfer, etc.

g) The work in the 3.6-m flame acceleration tube should be extended to other flammable mixtures, including hybrid mixtures (Skjold, 2013a) and combinations of gaseous or solid fuels and gaseous or solid suppressant agents. In light of the results presented in Publication M, it would be interesting to perform additional experiments with rich propane-air mixtures and initial turbulence.

h) The CFD simulations presented in Publication M indicate a significant effect of radiative heat transfer for explosion experiments in vessels of limited spatial scale. This phenomenon complicates the analysis of the experimental results with respect to comparative studies of dust and gas flames, since it is not straightforward to isolate the effect of varying degrees of heat losses to the wall and possible condensation of water vapour, from that of a thickened reaction zone or volumetric combustion behind the flame zone. Future studies should seek to clarify the effect of radiative heat transfer from the flame to the particles in the surrounding cloud.

i) Previous investigations of dust explosions ignited by weak ignition sources, in both 20-litre explosion vessels and transparent balloons, show that the rate of energy release during the initial phase of flame propagation in turbulent dust clouds can vary significantly, in spite of seemingly identical test configurations (Skjold, 2003; Skjold *et al.*, 2013). This phenomenon is likely a result of turbulent quenching. The apparently random delay in the onset of pressure rise in constant volume explosions complicates the analysis of experimental results, and hence reliable determination of important combustion parameters (Dyduch & Skjold, 2010; Dahoe *et al.*, 2013). Future investigations in this area should include measurements of dust concentration, radiative heat fluxes and turbulence parameters.

j) A likely reason for the discrepancy between experiments and simulations for rich propane-air mixtures is the fact that the combustion model in FLACS uses values for the laminar burning velocity S_L as the primary measure of reactivity. Ranzi *et al.* (2012) reviewed experimental data for laminar burning velocities for various hydrocarbons, and presented S_L data for propane in the concentration range 2.45-6.30 % (ER 0.6-1.6). It is not straightforward, or perhaps not even possible, to determine unambiguous values for S_L in propane-air mixtures for concentrations in the range 6.3-10 % (ER 1.6-3.0). This poses a challenge to combustion models that rely on empirical correlations for the turbulent burning velocity S_T, since even moderate levels of turbulence significantly alter the mode of flame propagation in fuel-rich propane-air mixtures (Skjold, 2003).

k) Further progress with respect to the use of advanced integral balance models for determining fundamental combustion properties for fuel-air mixtures can provide valuable input to CFD simulations with FLACS and DESC (Dyduch & Skjold, 2010; Dahoe *et al.*, 2002, 2013).

l) Validation of CFD codes for industrial applications requires high-quality validation data from repeated experiments.

Finally, the promising results obtained with CFD simulation, and the significant spread in results from large-scale dust explosion experiments, should have implications for design guidelines:

m) Future revisions of safety standards, such as EN 14491 (2006) and NFPA 68 (2013), should account for the uncertainty in experiments, and utilize results from CFD simulations in conjunction with experimental data to obtain consistent results (Tascón *et al.*, 2009, 2011).

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