The use of a CFD-model for predicting blast and fire ball effects due to vented dust explosions

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1 INTRODUCTION

The most common way to protect equipment from the consequences of dust explosions is venting. The method has, however, some drawbacks, viz. the generation of flame jets and the generation of blast waves endangering the direct surroundings of the vent.

Several research programmes have been carried out to develop guidelines to predict the secondary consequences of vented dust explosions. The research considers both hazards due to flame jets and blast effects generated by vented dust explosions. Examples are the work by Hattwig [1] and Wirkner-Bott et al. [2]. The results of the latter research work have been included in the latest issue of the VDI-guideline VDI 3673 [3]. The guideline allows for predicting the length of flames emerging from the vent opening and the strength of blast waves generated outside the vent opening both in the direction normal to the vent opening. A review of research work in this area was reported in [4].

In 1993 a 2 year EU-supported research project was started to investigate the secondary effects of dust explosions on a large scale and to develop models and improved guidelines in this area. As a part of this project Christian Michelsen Research developed a sophisticated model to describe blast and flame jets due to vented dust explosions. The model would allow for predicting directional effects, the effects of more than 1 vent opening and the possibility of protection of people and equipment by large walls at some distance of the vent opening.

This paper describes the results of this work. Starting from an existing CFD-model available for describing gas explosions in vented enclosures the work consisted of the following steps:

- development and implementation of a blast model
- implementation of a dust combustion model
- validation

First the CFD-model is described followed by a discussion of each step mentioned above. The capabilities of the model are demonstrated for one of the experiments used to validate the model.

2 SHORT DESCRIPTION OF THE FLACS-CODE

FLACS is a fluid dynamic code developed for description of gas dispersion and explosion processes in complex geometries such as offshore modules [5]. FLACS calculates explosion pressure and other flow parameters as a function of time and space for different geometries and explosion scenarios. It takes account of the interaction between flame, vent areas and obstacles such as equipment and pipe work. The FLACS code solves the full gas dynamic partial differential equations for a set of control volumes. The effects of turbulence and chemical reactions are included in the differential equations. The equations are discretised using a finite-volume technique and a weighted upwind/central differencing scheme for the convection terms. Velocities are calculated on staggered grids. The effect of turbulence is included through the eddy viscosity concept by solving equations for turbulent kinetic energy (k) and its rate of decay (ε).

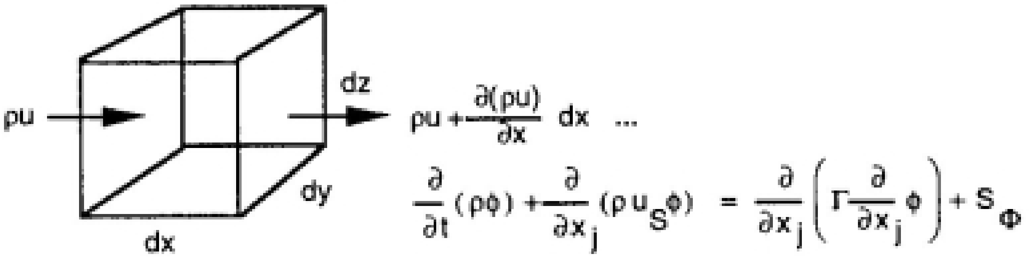


Figure 1 Partial differential equations solved in FLACS.

The FLACS code has well-developed pre- and post-processor programmes allowing for designing the explosion scenarios that have to be investigated and to produce output data.

3 IMPLEMENTATION OF A BLAST MODEL

The first necessary improvement of the FLACS-code in the present context was to describe accurately the propagation of generated blast waves into the surroundings and the interaction of these blast waves with nearby structures. Two distinctive developments were carried out:

- the use of a multi-block grid where one can use different solvers in the areas where an explosion takes place and there where only blast wave propagation and interaction takes place
- the use of a special solver for the simulation of the propagation of blast waves and their interaction with structures

The multi-block approach allows for extending the calculation domain only in those directions where one wants to know the consequences of blast waves. This limits the total calculation time of simulations. In addition to that one can use a special less-demanding solver for the areas where blast propagation takes place but where combustion does not interfere.

The special solver that was chosen for describing blast waves is a solution method known as FCT (Flux-Corrected Transport). FCT limits numerical diffusion, maintaining the character of shock waves, i.e. discontinuities will not be smeared out over the numerical grid.

The blast solver as such has been validated. An example is shown in Figures 2 and 3. Figure 2 shows an experimental set-up described in [6]. The set-up consists of two box-shaped obstacles placed in a shock tube. The obstacles were provided with pressure transducers at the positions 1-6 as indicated. The obstacles are 5 cm high and 5 cm wide and are placed 7.5 cm from each other. The obstacles are as long as the width of the shock tube. Pressure-time histories were calculated at each monitoring position. Figure 3 shows measured and calculated pressure-time histories at the positions 3 and 4. The Figure shows that the blast solver reproduces the measured pressure-time histories reasonably well. The main features of the pressure-time histories are reproduced. Each step and peak is either due to the initial shock wave or due to reflections in between the two boxes. If a finer grid would have been used in the simulations the resolution of each pressure spike in the simulations would have been better resulting in an even better resemblance of measured and simulated pressure-time histories.

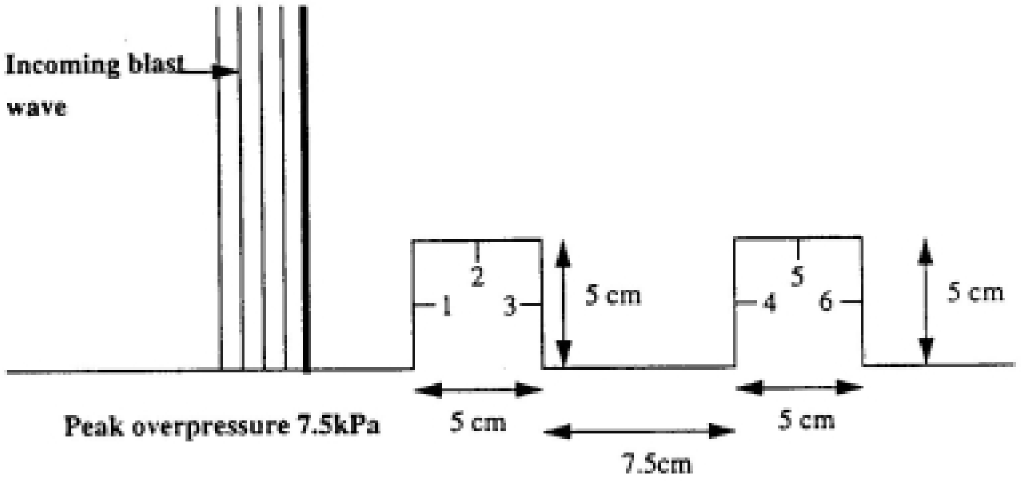
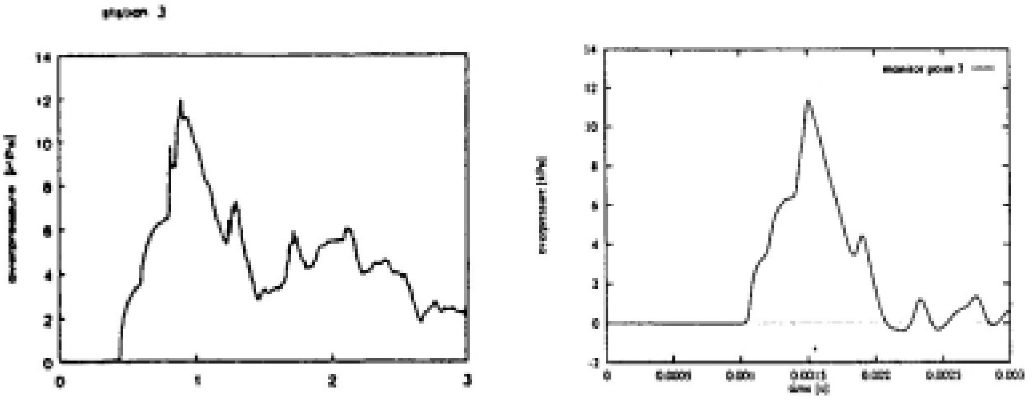
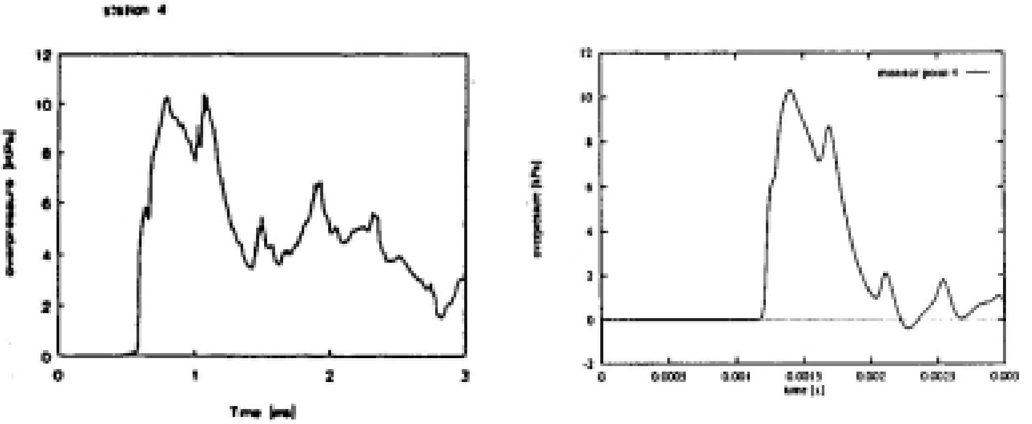


Figure 2 Laboratory-scale set-up used for studying blast-object interaction.



Experimental values of pressure-time histories at monitor point 3

Calculated pressure-time histories at monitor point 3



Experimental values of pressure-time histories at monitor point 4

Calculated pressure-time histories at monitor point 4

Figure 3 Calculated and measured pressure-time histories at positions 3 and 4 in the laboratory set-up shown in Figure 2.

4 INTEGRATION OF DUST COMBUSTION MODEL IN CFD-TOOL

4.1 Mechanism of flame jet and blast generation

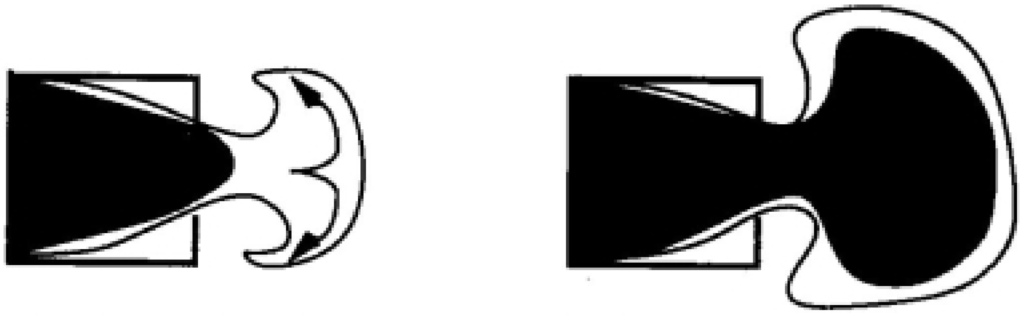
The mechanism of blast generation by vented dust explosions is closely related to the flame propagation processes in the vented vessel. Upon ignition combustion products are generated which will expand. The mixture in the vessel is compressed and the pressure will start increasing exponentially until the moment the vent cover starts to open. Due to the pressure difference over the vent opening the mixture in the vessel starts to flow out of the vessel. The outflowing mixture may be burned or unburned depending on the relative position of the ignition source and the strength of the vent cover.

In case of ignition far from the vent opening unburned mixture will be pushed out of the vent opening forming a jet. The jet velocity will depend on the size of the vent opening and the pressure in the vessel. At the edges of the opening and between the outflowing mixture and the stillstanding air outside the vessel turbulence is generated and a recirculation flow is established. This will cause entrainment of air and therefore dilution of the mixture. Mixtures of initially optimal concentration will therefore become leaner and less reactive. Rich mixtures will become more reactive.

The turbulent cloud of unburned mixture outside the vented vessel is ignited by the flame once combustion products are vented. For large vent openings this will lead to the generation of a more or less spherical flame ball. Due to the turbulence the flame speeds are very high resulting in strong blast waves. Small vent openings lead to very high jet velocities. As a result the mixture displaced from the vent is ejected a long way from the vent and the external flame propagation is elongated rather than spherical. A representation of the description given above is given in Figure 4. The most severe external effects appear to be determined by the external explosion.

a) start of outflow
unburned mixture

b) formation of jet head



c) flame approaches jet head

d) flame front becomes spherical

Figure 4 Several phases of the development of an external explosion.

Hence to be able to use FLACS to describe both flame jets and blast generated by dust explosions a model has to be implemented describing combustion of dust-air mixtures. This implies a model capable of describing the effect of pre-ignition and flame generated turbulence on dust combustion. Below the integration of a dust combustion model in the FLACS explosion tool is described. The integrated model has been validated against experiments performed in a 20 m^3 room.

4.2 Implementation of a dust combustion model

To be able to simulate gas explosions using the FLACS code a combustion model is used based on the flame library developed at Leeds University [7]. The same workers showed that a similar approach as accepted for gas explosions can be used for dust explosions [8]. Several institutions have been working on a dust combustion model describing the basic dust combustion properties as a function of turbulence parameters. Figure 5 shows an example of such research. The Figure shows the variation of the flame speed as a function of the turbulence intensity u’ for several dust-air mixtures (from [9]). The flame velocity increases linearly with the turbulence intensity. The data evolve from experiments performed in a 1.25 m^3 spherical bomb. Turbulence was generated by a pneumatic injection system.

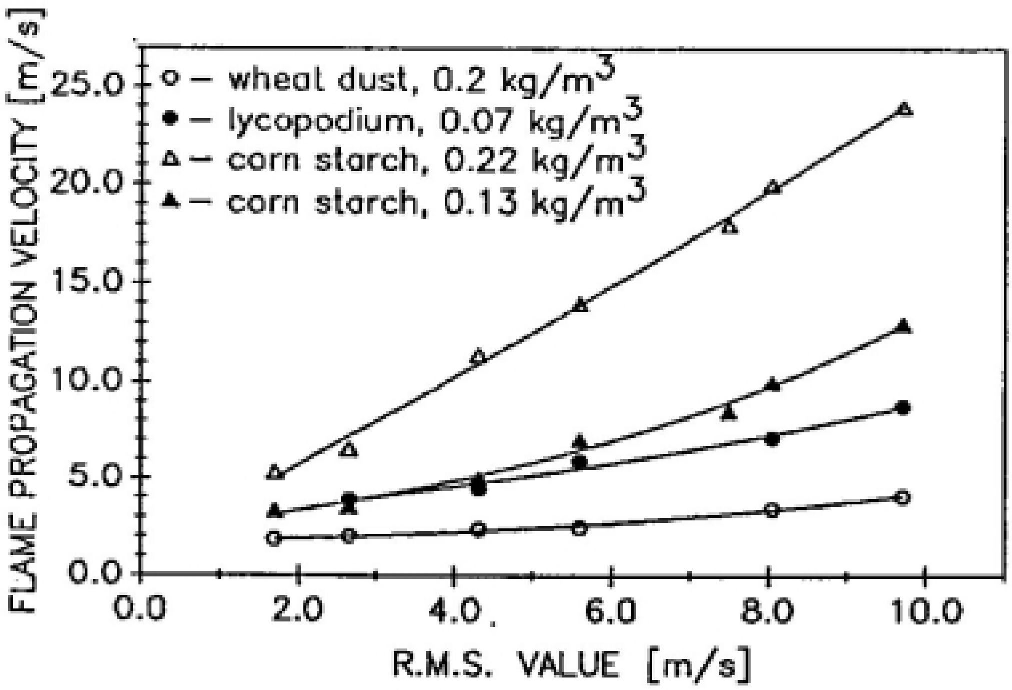


Figure 5 Effect of turbulence intensity u’ on the combustion rate of several dust-air mixtures (taken from [9]).

For gaseous fuels the linearity of the relationship breaks down at high turbulence intensities and may even lead to flame quenching. For dust-air mixtures one would expect a similar development and indeed quenching or flame speed reductions have been observed in intense turbulent flow fields. Examples are experiments performed in a channel where an intense turbulent flow field was generated by a fan [10] and explosions involving combustion generated turbulence in integrated systems [11, 12].

The gas and vapour combustion model described in [7] also takes the turbulence integral length scale into account.

A dust combustion model should take all these elements into account as well, i.e. effect of turbulence intensity, turbulence integral length scale on combustion rate and possibly quenching when the turbulence intensity is too high (for a given length scale).

The results shown in Figure 5, a linear increase of the combustion rate (expressed as a turbulent burning velocity (S_T) with turbulence intensity (u'), can be expressed in a single relationship:

$$S_T = S_L + Ku'$$

The coefficient K is a dust dependent coefficient: for maize starch a value of K=0.46 was found ([9]). It should be emphasised that the relationship does not account for the turbulent length scale: the K-value may differ for an industrial scale differing from the experimental scale.

S_L is the laminar burning velocity, the combustion rate in the absence of any turbulence. Also this parameter, should be measured. One way of measuring this parameter is in a tube closed at the top and opened at the bottom as described in. Dust is fed at the top, ignition is effected at the bottom. For maize starch measurements were reported in [9] and [13]. Table 1 presents the results.

Table 1 Laminar burning velocities measured for maize starch.

Dust type	Dust-air concentration (g/m^3)	Laminar burning velocity (m/s)
Maize starch [9]	700	0.59
Maize starch [13]	300	0.55

In addition to the combustion model, the aforementioned experiments performed in the 1.25 m^3 vessel allowed for the development of a model describing the effect of temperature and pressure on the turbulent burning velocity. Also this model was implemented in the CFD-tool. For maize starch the following relationship was found:

$$S_{T,T} = S_{T,0}(P/P_0)^0(T/T_0)^{1.7}$$

where $S_{T,T}$ = turbulent burning velocity at temperature T and pressure P
$S_{T,0}$ = turbulent burning velocity at temperature T_0 and pressure P_0

The relationship shows that the experiments revealed a strong temperature dependency and only a very minor pressure dependency.

4.3 Validation of code

The FLACS-code provided with the dust combustion model described above has been validated against experiments performed in a 20 m^3 room (dimensions 2.4 m x 2.4 m x 3.6 m) [14]. The room was provided with vent areas of 1 and 1.44 m^3 respectively. The very experiments were carried out with maize starch (concentration 750 g/m^3). The dust-air mixture was generated using the standardised way (ISO6184 [15]) of generating dust-air mixtures. Instead of ring-shaped nozzles, however, pepper boxes were used to disperse the dust and instead of a delay time of 600 ms a delay time of 900 ms was used. The vent opening was covered with a vent cover opening at a static opening pressure of 0.08 bar. The vent cover had a weight of 5 kg/m^2. Ignition was effected either in the centre of the room or at the rear wall.

The pressures were measured inside and outside the enclosure at several distances from the vent opening.

To be able to simulate these experiments several input parameters must be chosen such as:

- the degree of initial turbulence
- the laminar burning velocity of the fuel

To generate the dust cloud the dust was injected from pressurised hoppers in the roof of the test chamber. After a delay time of 900 ms ignition was effected. The degree of pre-ignition turbulence was not measured and therefore had to be estimated.

In [16] experiments are described where the turbulence intensity was measured in a 1 m^3 vessel while using the standard way of generating dust clouds [15]. The results show first of all that the turbulence is not isotropic as assumed when using a k-ε model in a numerical model to describe turbulence. The non-isotropic turbulence field is caused by the arrangement of the ring-shaped nozzle. The measurements revealed turbulence velocities of 1.2 m/s and 5.36 m/s for the two components that were measured (horizontal and vertical components respectively) at a delay time of 600 ms.

The experiments described in [15] were performed with an initial turbulence level controlled by adjusting the dust dispersion pressure and ignition delay. The adjustment was such that the internal overpressure obtained under the experimental conditions with central ignition was in accordance with the VDI 3673, nomograph approach [3]. This implied a delay time of 900 ms as mentioned above.

This would mean a turbulence intensity of 1.2 to 5.36 m/s assuming a similar turbulence length scale as in the 1 m^3 vessel. Regarding the use of isotropic turbulence in the k-ε model one can assume a turbulence intensity of 3.28 m/s.

The turbulence length scale will affect both the burning rate and the rate of turbulence dissipation. The combustion model described above does not describe the effect of turbulence length scale on the combustion rate and therefore cannot be taken into account directly. The rate of turbulence dissipation is of paramount importance for the course of the dust explosion since turbulence dominates the rate of combustion. The faster the rate of dissipation, the lower the overpressure generated in the 20 m^3 chamber will be. The rate of dissipation will determine the degree of turbulence at the moment of ignition but also during the combustion phase since the turbulence will continue dissipating. The rate of turbulence dissipation is closely related to the turbulence length scale.

The second parameter that has to be known to be able to use the model is the laminar burning velocity S_L. Results of measurements have been presented in Table 1. The 20 m^3 chamber explosion experiments were carried out for a concentration of 750 g/m^3. The laminar burning velocities were not measured for such a high concentration. On the basis of a relationship between K_{St}-value and dust concentration, however, a laminar burning velocity of S_L=0.7 m/s was chosen [13].

The correction for pressure and temperature increase during the course of the explosion was performed using the relationship developed by [7] and presented before.

For the simulations the main unknown factor is the turbulence at the moment of ignition. For the turbulence intensity a reasonable estimate could be made on the basis of 1 m^3 vessel turbulence measurements. The turbulence integral length scale, however, was calculated by the k-ε model. Starting from a turbulence intensity of 10 m/s and a length scale of 0.4 m (17 % of the smallest dimension of the room) the turbulence length scale reaches a steady value of approximately 2 cm. At a turbulence intensity of 3.3 m/s ignition is effected.

According to the k-ε model the turbulence intensity keeps on decreasing to a minimum value of approximately 2 m/s during the further course of the explosion. Depending on the location of the measurement of the turbulence intensity an increase is possible due to flow through the vent opening where turbulence is being generated due to the explosion itself towards the final stages of the explosion.

The first simulations of the experiments performed in the 20 m^3 room [14] showed that when applying the input parameters as described above the tendencies (effect of vent opening size, ignition point) were predicted well but the absolute values of the simulated pressures inside the room are too low in comparison to the experiments. The reason for this may be:

- a too strong dissipation of the turbulence in the simulations
- the ignorance of the effect of turbulence length scale on the burning rate in the combustion model that has been applied
- a combination of these factors

It was assumed that the relative difference was due to the second factor. To allow for the effect of a larger turbulence length scale, the K-factor in the combustion model was increased from K=0.46 to K=0.8. The results of simulations using this adapted combustion model can be shown in Table 2.

Table 2 Results of simulations of dust explosions in a vented 20 m^3 chamber using maize starch.

ID	Vent opening size (m2)	Ignition location	Internal overpressure (bar)	Blast (0.5 m) (mbar)	Blast (2.5 m) (mbar)	Blast (5m) (mbar)	Blast (10 m) (mbar)	Blast (15 m) (mbar)	Blast (20 m) (mbar)
Simulation	1.44	rear	0.38	41	74	99	57	32	23
Experiment	1.44	rear	0.33-0.35	51-66	35-57	93-140	23-67	34-67	9-31
Simulation	1.44	centre	0.28	17	48	34	25	16	8
Experiment	1.44	centre	0.2-0.25	33-34	42-51	44-51	6-19	20-30	4-15
Simulation	1.0	centre	0.63	30	120	134	170	123	-
Experiment	1.0	centre	0.66	53	54	38	30	26	14

Simulated pressure-time histories are presented in Figure 6.

The simulation results show the possibilities of the CFD-code. The internal overpressures are well reproduced within the reproducibility of the experiments. The external overpressures are reproduced as well for the larger vent opening. For the smaller vent opening a clear overestimation of external overpressures by the model is found. This may be due to local quenching in the flame outside of the vent opening. Due to the higher pressures inside the room combined with the smaller vent opening flow velocities and therefore turbulence intensities will be very high possibly causing local quenching. For the larger vent opening case quenching does not occur. In the combustion model this is not taken into account. The reduced combustion rate results in the generation of less strong blast waves.

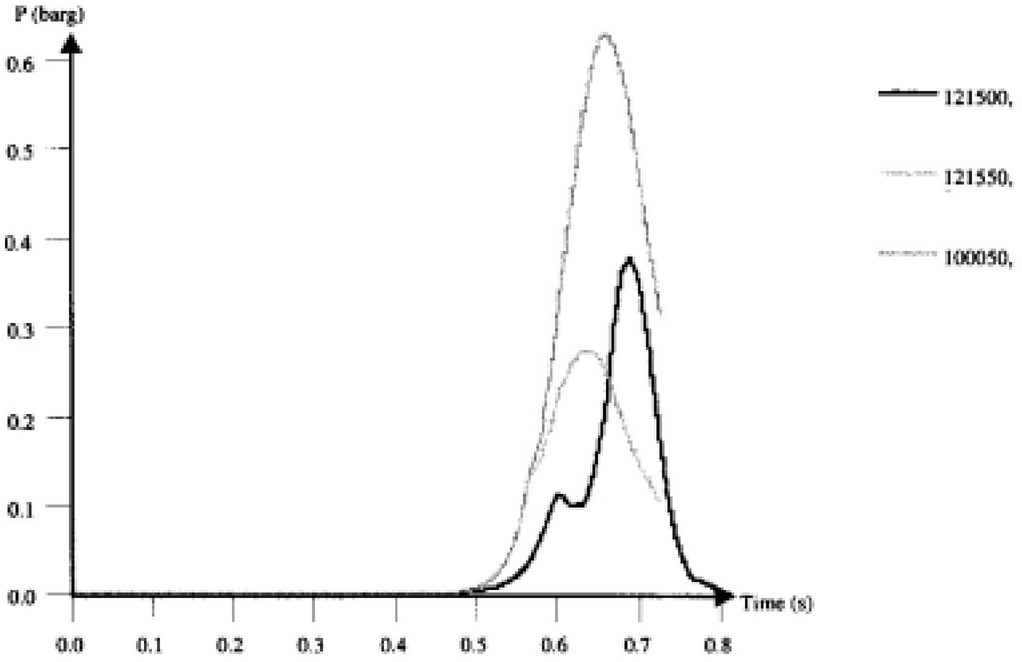


Figure 6 Simulated pressure-time histories measured inside the 20 m^3 room for maize starch-air explosions (121500 = rear wall ignition, 1.44 m^2 vent opening; 121550 = central ignition, 1.44 m^2 vent opening; 100050 = central ignition, 1.0 m^2 vent opening).

The size of fireballs was in general slightly underestimated. The maximum flame length was approximately 25 m in the experiments whereas the simulations predicted maximum flame lengths of 18 m.

One can therefore conclude that provided a dust combustion model is developed capable of taking into account all the effects turbulence may have on combustion (combustion rate increase and local quenching) depending on turbulence intensity and length scale it will be possible to use CFD-models to predict the consequences of dust explosions including the internal overpressures and blast effects and fire balls due to vented dust explosions.

The present work also shows that there is a great need for suited validation experiments.

5 CONCLUSIONS

An existing CFD-model available for prediction of gas explosions has been adapted to allow for prediction of the secondary consequences of vented dust explosions.

To this end the model was extended by implementing

- a blast model
- a dust combustion model

The blast model is based on the FCT-algorithm optimising numerical diffusion to maintain the shock-wave character of blast waves. The model was validated against experiments concerning the interaction of a shock wave with box-shaped obstacles in a shock tube.

A dust combustion model based on experiments performed in a 1.25 m^3 vessel was implemented. The model takes into account the effect of turbulence intensity on the burning rate as well as the effect of increase of temperature and pressure.

A validation against dust explosion experiments carried out in a 20 m^3 vented chamber highlighted that provided a dust combustion model is developed capable of taking into account all the effects turbulence may have on combustion (combustion rate increase and local quenching) depending on turbulence intensity and length scale it will be possible to use CFD-models to predict the consequences of dust explosions including the internal overpressures and blast effects and fire balls due to vented dust explosions.

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