A.1 Modeling and image analysis of FAE

(13 pages)

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Introduction

Fuel-air explosives (FAE) are typically liquid fuel dispersed in air by a high explosive charge to make a fuel-air cloud that is detonated. Modeling the FAE detonation wave and the subsequent shock propagation in air can be handled by different methods. In [1] the detonation properties are imposed on a front that propagates with the detonation velocity. A simpler method is to assume constant volume combustion. In this paper an alternative method for simulating detonations in fuel-air mixtures is presented. This method is based on a temperature dependant reaction rate and it was developed for simulation of deflagration and detonation in gas-air mixtures [2]. There are different numerical schemes for handling nearly discontinuous solutions. In this paper a centered total variation diminishing (TVD) scheme is used. These numerical schemes are simpler and faster than upwind TVD schemes, but may introduce more numerical diffusion. For validation of these methods for large scale explosions results from simulations are compared with experiments, both free field and in complex geometries. Free field experimental results are taken from the propylene-oxide tests in the Elk Velvet 2, 3 and 4 trials performed at DRDC at Suffield, Canada in 2005, 2006 and 2007 [3],[4],[5]. The tests with a complex geometry are taken from the Elk Velvet 4 trials. Simulation results are also compared with pressure records and extracted pressure data from the high speed films of the explosions. This technique gives an almost continuous pressure-distance relationship for the shock wave. The objective of this work is to test the numerical scheme with the reaction rate model and compare the simulated pressure and impulses with experimental results of the Elk Velvet FAE trials.

Reaction Models

There are three species in the system, reactants, products and air. A reaction progress variable describes the reaction of propylene-oxide and air and the transport of reactants and products, equations 1 and 2. A passive variable is transported to include air as the third component.

$$\frac{\partial \rho \beta}{\partial t} + \nabla \cdot (\rho \vec{u} \beta) = -\rho \dot{\omega} \tag{1}$$

The reaction rate is described by an Arrhenius type reaction term.

$$\dot{\omega} = A \rho^{0.5} \beta^{1.5} exp\left(-T_a / T\right) \tag{2}$$

Here β is a reaction progress variable, ρ is the mass density, the vector u is the velocity vector, A is a pre-exponential factor, Ta is an activation temperature and T is the gas temperature. The pre-exponential factor A = 4.107 m1.5/(kg0.5s) and activation temperature Ta = 15000 K where chosen to give the detonation velocity and the CJ-state with a 1D detonation of propylene-oxide and air. A different and simpler way of calculating the source is to assume the whole cloud is burned as a constant volume process. The initial conditions are the products of a constant volume process with a constant pressure, calculated from equation 3, and a heat capacity ratio for the products set in the cloud volume.

$$p_{CV} = (\gamma_{CV} - 1)\left(q + \frac{p_0}{\gamma_0 - 1}\right) \tag{3}$$

Here q is the released heat pr. unit volume, p_{CV} is the constant volume combustion pressure, γ_{CV} is the heat capacity ratio of the products burned by a constant volume reaction, p_0 is the ambient pressure and γ_0 is the heat capacity ratio of the cloud.

Pressure Records

The pressure sensors used in the experiments are all piezoresistive sensors from Kulite. The free field transducers are placed in a 0.4 m X 0.4 m aluminum plates. The logging speed was 65.536 kHz/channel. More detail from the Elk Velvet 3 trials can be seen in [7].

Image Analysis

The image analysis of the high-speed film of the experiments are based on background oriented schlieren (BOS). This method is described in more detail by Sommersel et. al. [8]. The principle can be seen in Figure 1, where an unperturbed image is subtracted from a perturbed image to produce an image where the shock wave is seen more clearly. The position of the shock wave can then be extracted and with a logarithmic transformation and curve fitting the shock Mach-number can be found. The curve fitting of the position is done with the Matlab polyfit script. The shock pressure can be calculated from the normal shock relations as shown in equation 4.

$$\frac{\Delta p}{p_0} = \frac{2\gamma}{\gamma + 1}\left(M^2 - 1\right) \tag{4}$$

Figure 1: The principle of the BOS-technique, the first image is a frame from the high speed movie with an vaguely visible shock, the second image is an unperturbed image and the third image is the difference of the two first images with a clearly seen shock wave.

Numerical and experimental set-up

Explosions in two different geometries has been simulated. One geometry is two-dimensional (2D) axis symmetric sylindrical shown in Figure 2. This is for comparison with free field measured pressures. The other geometry is a three-dimensional (3D) Cartesian with a structure shown in Figure 3 and computational domain shown in Figure 4. Initial pressure and temperature in the experiments was 92.2 kPa and 281 K for all experiments. The detonation was initiated by a high explosive charge placed approximately 1 m above ground, this is simulated by a high pressure and temperature region. The two explosive sizes of 55 kg and 166 kg of propylene-oxide gives different cloud sizes, the approximate size of the clouds is taken from the film of the experiments. The size of the cloud is also the basis for the calculation of the released energy pr. mass. The cloud is assumed to be pancake-shaped. For the case with 55 kg of fuel the radius of the cloud is 6.8 m and height of the cloud is 2.8 m. For the 166 kg cloud the radius is 9.8 m and the height is 3.9 m. The thermodynamic package SuperSTATE is used to calculate the heat release, q and thermodynamic properties of the species, for the average homogeneous stoichiometry of the cloud.

Free Field

Results from simulations with 2D axis symmetry are compared with free field pressures. Figure 2 shows the computational domain, with the two simulation directions radial, r and axial, z. The radial axis, at z = 0 is the ground. Two different mesh sizes is used to test the grid dependency of the method, 5 cm in r and z direction and 10 cm in both directions. These tests are done with a fuel mass of 55 kg.

Container Observation Post (COP)

The computational domain with the initial FAE cloud is shown in Figure 3. The center of the gas cloud is placed 20 m from the center of the Container Observation Post (COP). The figure shows the domain in the horizontal plane with outer boundaries. The two boundaries normal to X-Y directions are the bottom and top boundaries. The bottom boundary is a wall (ground) and the top is set to a zero gradient boundary. Length X is 28 m, width Y is 40 m and height Z, normal to the X-Y is 20 m. The spacing of the computational mesh for the cases with COP is 0.2 m in all directions. Experiments and simulations are done with both 55 kg and 166 kg of fuel. In Figure 4 the geometry of the structure and the position of the pressure transducers is shown. This is how the geometry is in the simulations however there are some small differences from the real structure. Figure 5 shows an image of the geometry.

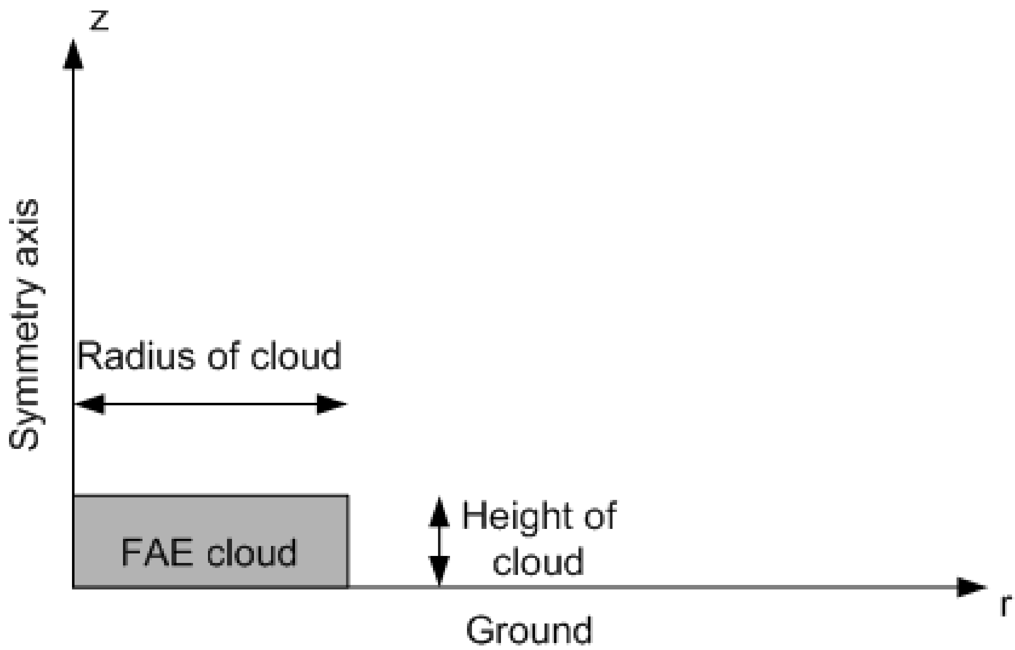

Figure 2: Computational domain for two dimensional axis symmetric calculations.

Results

Free Field

The results from the free field simulations are presented as shock pressure and positive impulse as a function of a reduced length. The reduced length is distance from the center of the cloud divided by the cubed root of the ratio of theoretical released energy, E0 and ambient pressure, p0. The released energy is the product of the heat of combustion and the mass of propylene-oxide, E0 = Hc.mfuel. Where Hc is 30 MJ/kg and mfuel is 55 kg or 166 kg. This scaling is the same as for the TNO multi-energy method [9]. The Simulation 5 cm mesh, 55 kg is simulation results of 55 kg of propylene-oxide with 5 cm mesh spacing. The same notation is used for the other cases. The Constant Volume graph is the constant volume combustion products initial conditions with 5 cm mesh spacing. The experimental results shown in Figure 6 and Figure 7 are experiments with 55 kg and 166 kg of mass. Figure 6 displays the shock front pressure and Figure 7 shows the maximum impulse.

Figure 8 shows results of the free field experiments together with a 2D

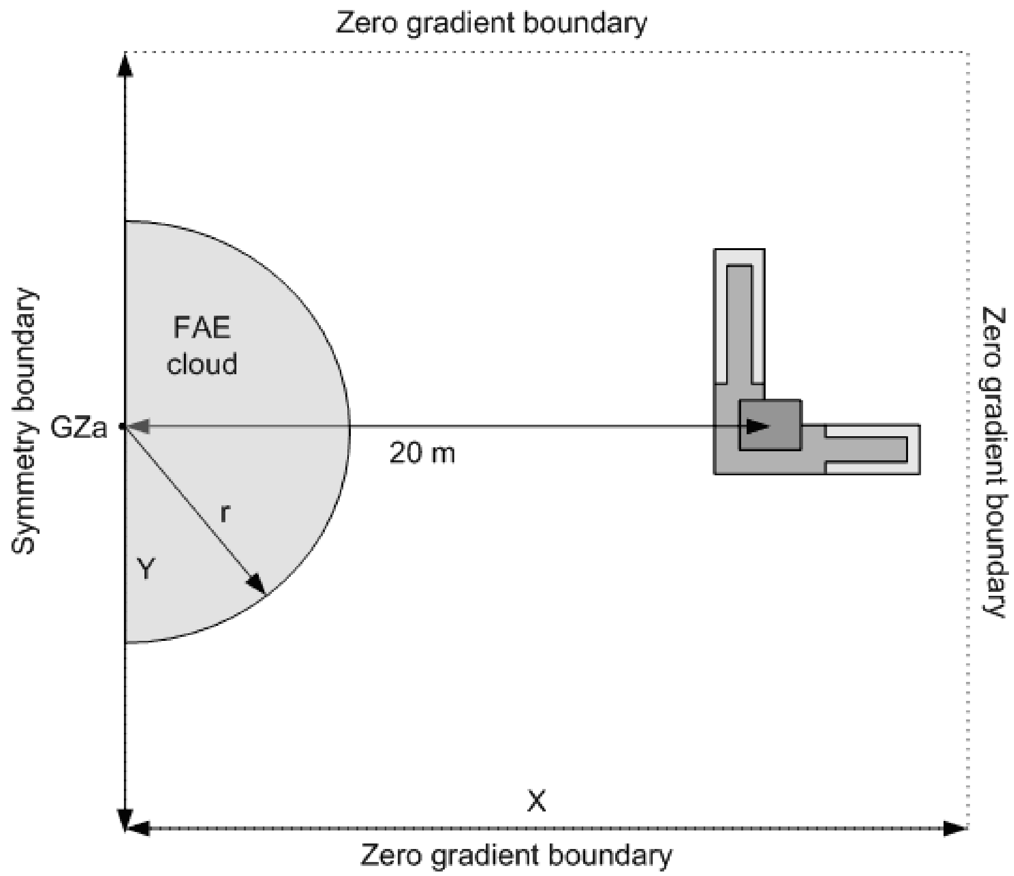

Figure 3: Horizontal plane of the computational domain for the 3D geometry with boundary conditions.

simulation of 55 kg fuel and the predicted pressure from the image analysis method. The 2. order and 3. order curves are for 2. and 3. order interpolation of the Mach-number based on shock positions from the high-speed movies. The 2. and 3. order interpolation of the 55 kg experiment are indistinguishable. For the experiments with 166 kg, the front of the COP started at a reduced distance of approximately 0.65. The shock interacts with the COP at this distance and will contribute to the discrepancies between the 2. order and 3. order interpolation of the position and between the 166 kg and 55 kg cases.

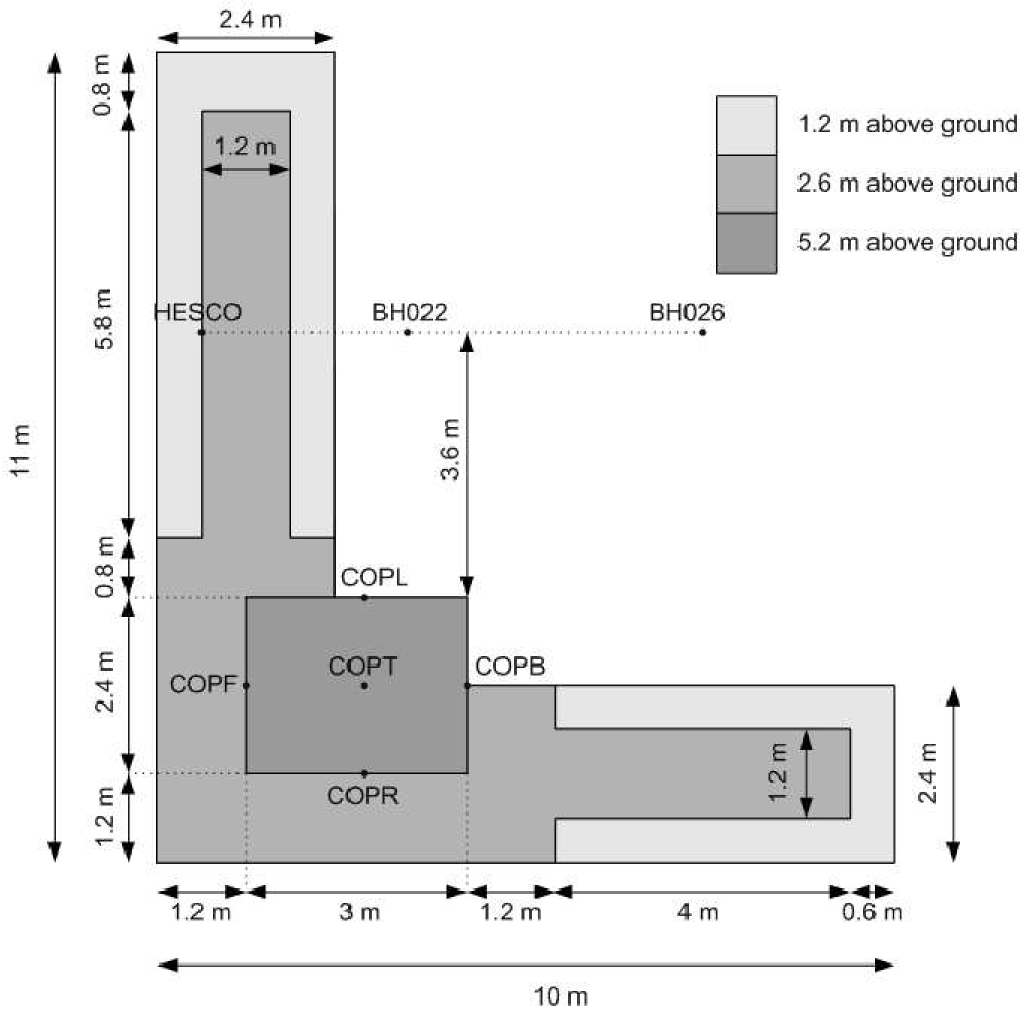

Figure 4: The COP geometry with positions for pressure transducers.

COP

Figure 9 and Figure 10 shows experimental and 3D simulated pressure and impulse as a function of time at the COPF pressure transducer, see Figure 4 for details.

For comparison of experiments and simulations Table 1 and Table 2 displays the maximum pressure and impulse for all pressure transducers. Table 1 is for 55 kg of fuel and Table 2 is for 166 kg of fuel, see Figure 4 for details on the positions of the transducers.

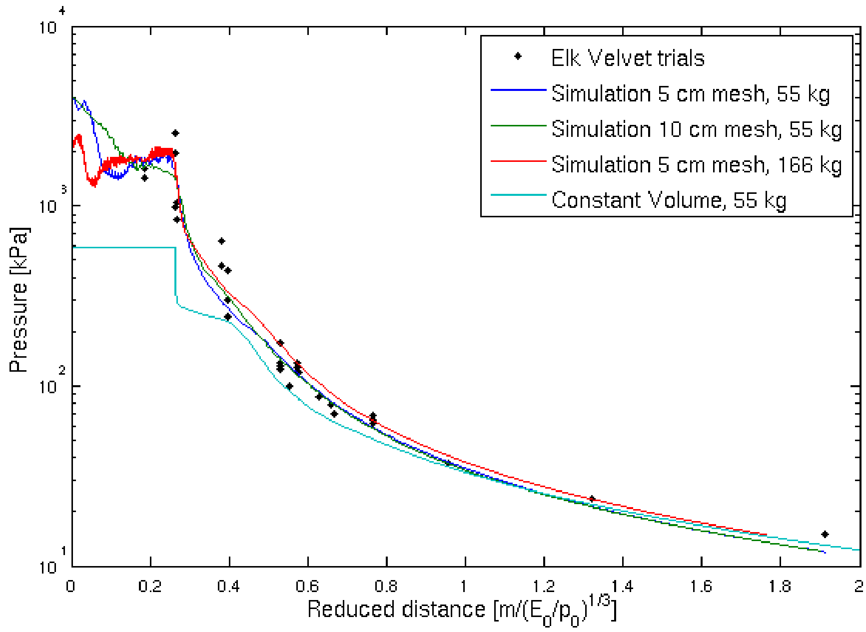

Figure 5: Simulated (2D) and experimental shock pressure along the reduced distance, scaled by energy. The Elk Velvet trials and are either 55 kg or 166 kg of propylene-oxide.

Table 1: Maximum pressure and impulse from experiments and simulations with 55 kg propylene-oxide.

Pressure Transducer	Pressure experiments [kPa]	Pressure simulations [kPa]	Impulse experiments [kPa · ms]	Impulse simulations [kPa · ms]
HESCO	160	163	776	772
BH022	30	25	327	302
BH026	28	28	315	307
COPF	170	154	723	693
COPL	53	49	230	262
COPR	52	50	323	342
COPB	29	24	315	267
COPT	42	44	328	334

Discussion

The free field 2D simulations in Figure 6 and Figure 7 show good agreement with the experiments. The simulated shock pressure is lower than the exper-

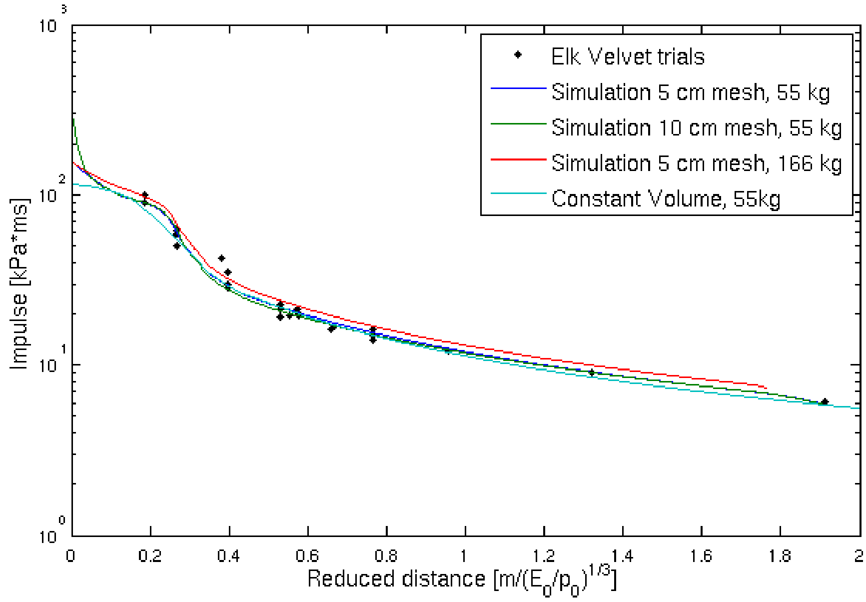

Figure 6: Simulated (2D) and experimental maximum impulse along the reduced distance, scaled by energy. The Elk Velvet trials and are either 55 kg or 166 kg of propylene-oxide.

Table 2: Maximum pressure and impulse from experiments and simulations with 166 kg propylene-oxide.

Pressure Transducer	Pressure experiments [kPa]	Pressure simulations [kPa]	Impulse experiments [kPa · ms]	Impulse simulations [kPa · ms]
HESCO	536	466	1820	1768
BH022	64	52	609	543
BH026	72	61	593	572
COPF	404	394	1524	1484
COPL	115	98	603	579
COPR	122	99	371	403
COPB	57	39	589	477
COPT	95	82	605	536

imental pressure far away from the source. This is likely due to numerical diffusion as the pressure peak is smoothed over a few control volumes. This effect is not seen in the impulse, as the energy is not dissipated due to the

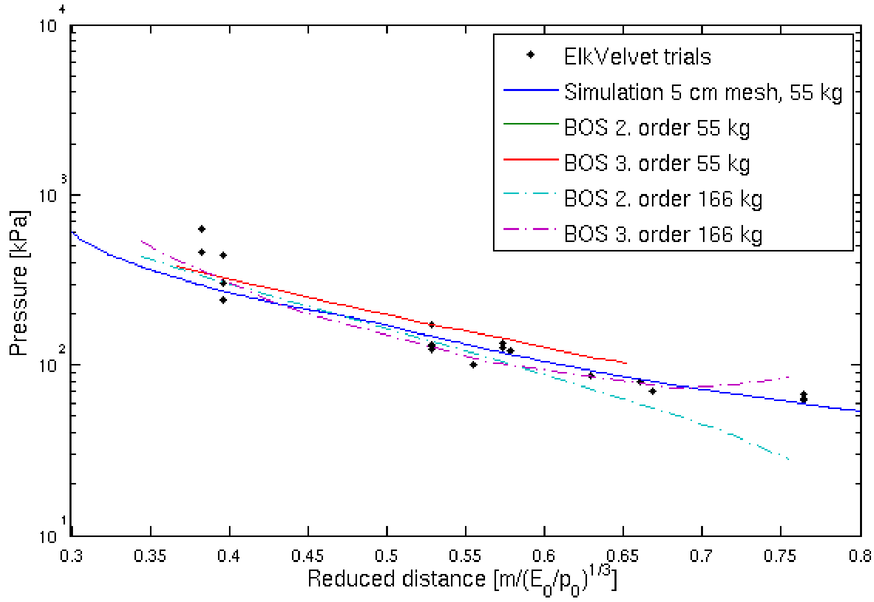

Figure 7: Free field experimental data together with simulations of a 55 kg FAE and results from the image analkysis. The 2. and 3. order interpolation for 55 kg are equal and can not be distinguished.

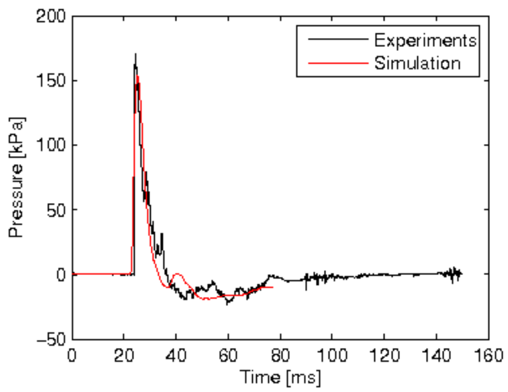

Figure 8: Experimental and simulated pressure history at pressure sensor COPF for 55 kg of propylene-oxide.

numerical diffusion. The mesh size does not seem to effect the performance too much for the 2D axis symmetric simulation. The 166 kg cloud produce stronger shock, based on the cloud sizes this cloud is richer than the 55 kg

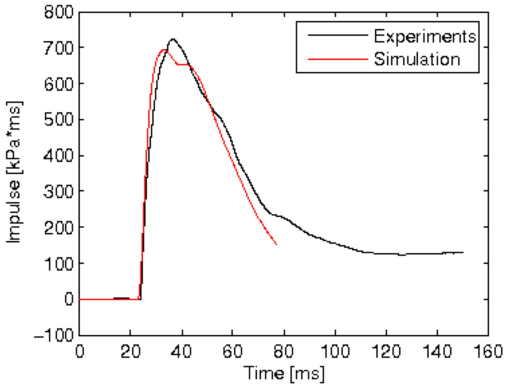

Figure 9: Experimental and simulated impulse history at pressure sensor COPF for 55 kg of propylene-oxide.

cloud, and the mixture is closer to the CO stoichiometric concentration on average. The released energy pr. unit volume is therefore higher for the 166 kg cloud than for the 55 kg cloud. By setting the same initial FAE cloud volume as a constant volume combustion products state the results are quite good compared with the experimental results. The pressures are in some degree under-predicted near the cloud but the impulse is equally good as for the reaction rate. For a system like this where there are no structures within the FAE cloud, the constant volume method might be as good a method as a reaction rate model. The reaction rate model may handle shock reflections and more complicated wave structures in the cloud but this may not be important in many cases. The image analysis is taken from high speed films of the shock close to the COP, for the 166 kg FAE the shock was above the walls of the COP and the results after a reduced length of 0.65 is not comparable to the free field data as presented in Figure 8. The extracted shock pressure from the high speed films are in good agreement with simulation data and experimental pressure records. For the three dimensional simulations the pressure and impulse show a good agreement with experiments. Figure 9 and Figure 10 and Table 1 and Table 2 shows the results for these experiments and simulations. The strength, time of arrival and the duration of the blast wave is reproduced in the simulations, with some discrepancies in the pressure history. The secondary shock is predicted later than in the experiments and is then seen in the negative phase. This might be a numerical diffusion problem and in this case the mesh is coarse. Since the predicted impulse follows the experimental impulse quite well this is probably not too important for the analysis.

Conclusion

The 2D and 3D simulation methods described in this paper can reproduce the loading from blast waves from FAE. The predicted pressures and impulses are in good agreement with the experimental results both for the free field experiments and for the tests with a COP. Some effects from numerical diffusion are seen in the far field pressures, but the impulse is not affected by this. The constant volume combustion source gives reasonable results for the impulse but the pressure is under-predicted near the cloud. The image analysis based on BOS is also able to reproduce experimental pressures from a high speed film of a shock wave and may also be helpful in validating CFD methods. We conclude that the FLIC scheme with the reaction rate model can produce pressure and impulses that agrees quite well with experimental results of fuel-air explosives.

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