MODELING OF GASEOUS EXPLOSIONS IN CONFINED AND UNCONFINED VOLUMES

Sharad Gupta[1], Abinash Baruah[2], Vidhuresh S[3], and Anil Kumar K. R.[4]

[1]Fluidyn Software, No. 146, Sector 5, H.S.R. Layout, Bangalore – 560102
[2]Dept. of Space Engg. and Rocketry, B I T, Mesra, Ranchi – 835215
[3]Fluidyn Software, No. 146, Sector 5, H.S.R. Layout, Bangalore – 560102
[4]Fluidyn Software, No. 146, Sector 5, H.S.R. Layout, Bangalore – 560102, anil.kumar@fluidyn.com

ABSTRACT

A proper estimate of the formation of an explosive gaseous cloud in a partially confined mining system is one of the essential factors in designing the mine configuration and its ventilation systems. Also, an accurate knowledge of the pressure-wave generation and propagation due to the explosion of a reactive cloud helps in deciding the safeguards in the event of an accident. In the present work a numerical model has been developed to compute the generation and dispersion of explosive gases and hazardous pollutants and possible fire and explosion due to them inside a mine environment. It computes the transient flow fields by solving the three-dimensional conservation equations for the momentum, energy, and species using a finite volume method. It can handle the turbulent flow of gas mixtures and the dispersion of gases through an interconnected network of tunnels, ducts and mine shafts. To accurately model the fire and explosion of reactive mixtures under different conditions, various combustion models have been included.

This paper presents the results of two studies done to validate the explosion models. In both the studies the temporal variation of the computed overpressures at different monitor points are compared with the experimental measurements. The first study concerns an unconfined explosion leading to the detonation of a premixed methane-oxygen cloud in an open atmosphere. The second study deals with the burning of a premixed methane-air cloud in a specially constructed, partially vented chamber resulting in an almost confined explosion.

KEYWORDS: *CFD*; *Gaseous Explosion*; *Unconfined Detonation*; *Pressure-Wave Propagation.*

1. INTRODUCTION

The current mining activities require high productivity with equal emphasis on the safety and health of the employees. This requires adequate estimation of the risks arising from different sources to the people and equipments. Generation, dispersion, and accumulation of reactive gases form one such source. A premixed cloud of gaseous reactants, such as methane, and air could lead to an explosion and/or detonation when ignited with sufficient energy. This can lead to very strong pressure waves, which are dangerous to people and the mine system. A proper estimation of the formation of an explosive cloud in the confined environments of mines requires an accurate computation of both, the flow field and the dispersion of different species in a confined environment. In the present work a numerical model, which is being included in the computer program Fluidyn-VENTMINE, that is specially designed to analyze transport phenomena in mines, has been developed to model the generation and dispersion of explosive gases and hazardous pollutants, and possible fire, explosion, and detonation due to them inside a mine environment. It can handle the turbulent flow of gas mixtures and the dispersion of gases through an interconnected network of tunnels, ducts and mine shafts. The computation of pressure-wave generation and propagation due to an explosion in a confined environment poses many difficulties due to inherent non-linear nature of the combustion process and its strong dependence on the turbulence. Hence, to accurately model the fire and explosion of reactive mixtures, various combustion models such as the Arrhenius model, the Eddy Dissipation model, the standard Bray-Moss-Libby (BML) model and the Hybrid Kinetic-Mixing model have been included. This paper presents the results of two studies done to validate the combustion and pressure wave propagation models in Fluidyn-VENTMINE.

In this paper, Section 2 describes the physical problems considered, Section 3 briefly explains the general method of solution and Section 4 presents the computational results and comparison with experimental measurements.

2. PHYSICAL PROBLEM

Two different scenarios have been considered. The first one deals with an unconfined explosion leading to the detonation of a premixed methane-oxygen cloud in an open atmosphere. This has been used to validate the model for explosions in an almost open domain. The second scenario concerns the burning of a premixed methane-air cloud in a specially constructed, partially vented chamber resulting in an almost confined explosion. This demonstrates the applicability of the model in much more severe conditions with multiple reflections of the pressure wave from the walls and release through small vents.

2.1 Problem 1: Unconfined Explosion

This problem consists of a spherical balloon filled with a mixture of methane and oxygen with an equivalence ratio of 1 (Kim *et al*, 2008) as shown in Figure 1. The initial pressure and temperature were 119.6 kPa and 281.05 K, respectively. The center of the balloon was 0.675 m above the ground. This mixture was ignited such that it led to detonation and the overpressures were measured at distances of 1, 2, 5, 10, 15, and 18 m, respectively, from the centre of the balloon, in the horizontal plane parallel to the ground.

2.2 Problem 2: Confined Explosion

This consists of an explosion of a mixture of methane and air. Figure 2 shows the experimental set up (Janovsky *et al*, 2003). Experiments were conducted in an experimental mine, which is 300 m long. Two masonry dams were built in the mine with a cross-sectional area of 10.2 m^2 separated by a longitudinal distance of 5.75 m, giving an explosion chamber of volume 58.65 m^3. Initially this chamber was partially filled with a mixture of methane and air that was ignited with a weak source. The initial laminar flame accelerates due to the inherent flow instabilities and the turbulence generated by the wall roughness. Eventually, it led to an explosion causing overpressures in the range of 0.1 bar to 1 bar. Explosions with different volumes and equivalence ratios of the reacting mixture and different vent areas were studied.

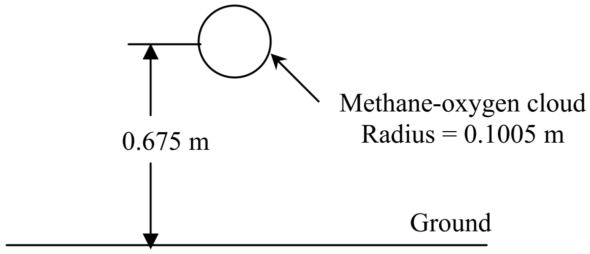

Figure 1: Schematic of the domain for problem 1.

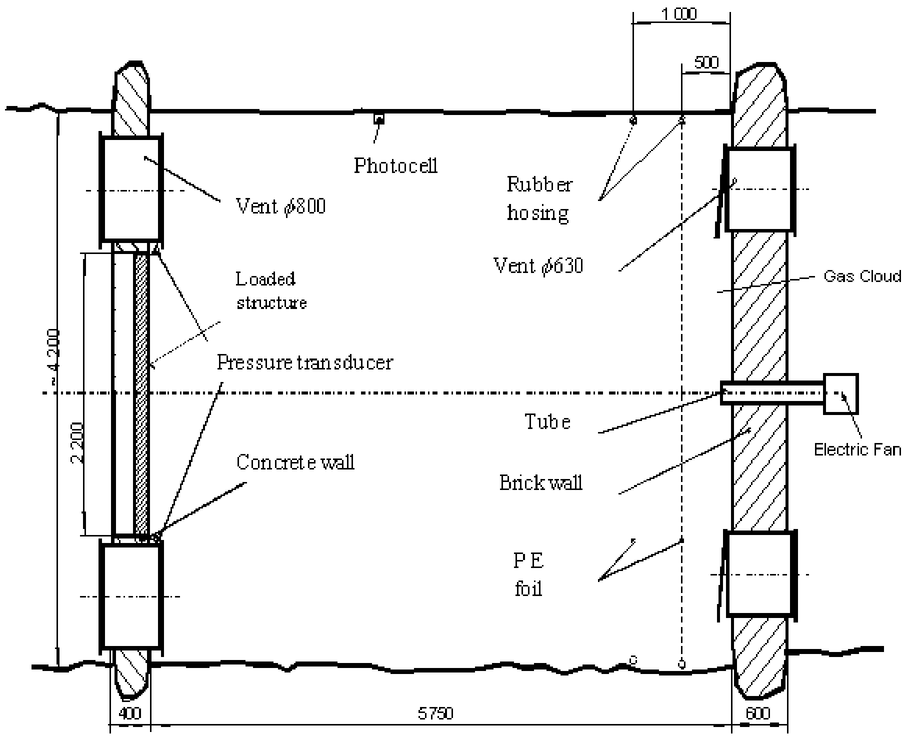

Figure 2: Schematic of the experimental set up for problem 2

3. METHOD OF SOLUTION

This section gives a brief description of the reaction and computational models used. The turbulent reacting flow fields, dispersion of different gaseous components and the resulting overpressures in the fluid, due to deflagration and/or detonation, are calculated by solving the conservation equations for the mass, momentum, energy, and species in a 3-dimensional framework using a semi-implicit, pressure-based, finite volume method. The computational model incorporates a wide range of deflagration, detonation and/or turbulence models and can handle multiple-species, multi-step chemical reaction schemes. The methodology for the evaluation of the source terms due to the chemical reactions is given below.

The chemical reactions occurring in the system are symbolized by

$$\sum_m a_{mr} x_m \leftrightarrow \sum_m b_{mr} x_m \tag{1}$$

where, x_m represents one mole (or chemical symbol of the molecule) of species m and a_{mr}, and b_{mr} represent integral stoichiometric coefficients for the reaction r. The stoichiometric coefficients must satisfy

$$\sum_m \left(a_{mr} - b_{mr}\right) W_m = 0 \tag{2}$$

where, W_m is the molecular weight of species m.
The chemical source term in the species continuity equation (1) for species m, for the Arrhenius reaction model is given by

$$\dot{\rho}_m^c = W_m \sum_r \left[\left(b_{mr} - a_{mr}\right) \dot{\omega}_r \right] \tag{3}$$

where, $\dot{\omega}_r$ is the rate of the reaction r.

For the BML model, the species source term is

$$\dot{\rho}_m^c = \sum_r \left[\Delta y_{mr} \dot{\omega}_r \right] \tag{4}$$

where Δy_{mr} is the initial mass fraction for the reactants and the possible mass fraction for the products after complete combustion.
The chemical heat release term (energy source term) in the energy equation, for the Arrhenius model is given by

$$\dot{Q}^c = \sum_r Q_r \dot{\omega}_r \quad . \tag{5}$$

For BML model, the energy source term is given by

$$\dot{Q}^c = \sum_r Q_r \Delta y_{fr} \dot{\omega}_r / W_{fr} (a_{fr} - b_{fr}) \tag{6}$$

where, Q_r is the negative of the heat of the reaction r at absolute zero and is given by

$$Q_r = \sum_m \left[\left(b_{mr} - a_{mr}\right) \Delta h_{fm}^0 \right] \tag{7}$$

where $\Delta h°_{fm}$ is the heat of formation of species m at absolute zero, and subscript f represents the reference species, which is normally fuel.

In the Arrhenius model the reaction rate, $\dot{\omega}_r$ is computed as

$$\dot{\omega}_r = k_{fr} \prod_m \left(\rho_m / W_m\right)^{a'_{mr}} - k_{br} \prod_m \left(\rho_m / W_m\right)^{b'_{mr}} \quad (8)$$

where, a'_{mr} and b'_{mr} are the reaction orders (reaction orders need not be same as a_{mr} and b_{mr} , so that empirical reaction orders can be used), k_{fr}, and k_{br} are the reaction coefficients of the forward and backward reactions, and ρ_m is the species density. The reaction coefficients are assumed to be of a generalized Arrhenius form:

$$k_{fr} = A_{fr} T^{\zeta_{fr}} e\left(-E_{fr}/T\right) \text{ and } k_{br} = A_{br} T^{\zeta_{br}} e\left(-E_{br}/T\right) \quad (9)$$

where, E is the activation temperature, A is the pre-exponential factor, ζ is the temperature dependence parameter, and T is the temperature.

In the BML model used, the reaction rate is calculated as (Bray, 1996)

$$\dot{\omega}_r = \rho_u S_L I_0 \Sigma \quad (10)$$

where, ρ_u is the density of the unburned mixture, S_L is laminar flame speed, I_0 is the stretch factor, and Σ is the flame surface density.

4. RESULTS

4.1 Problem 1: Unconfined Explosion

Figure 3 shows the computational domain and the locations of the pressure monitoring points. Figure 4 shows the computational mesh used; it is two-dimensional spherical. The mesh used is very fine, about 0.5 mm, in the gas cloud and is progressively coarsened away from the cloud. The flow is assumed to axis-symmetric about an axis normal to the ground. Arrhenius model with standard single step kinetic parameters is used for combustion.

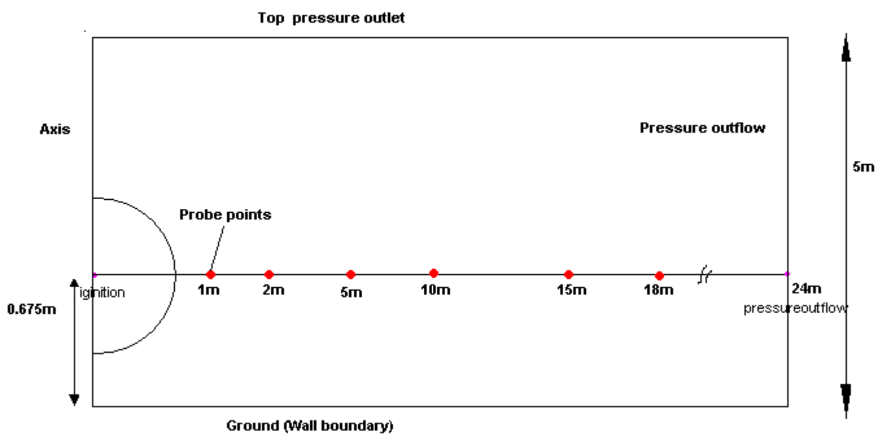

Figure 3: Computational domain and the pressure monitoring points for Problem 1 (not to scale).

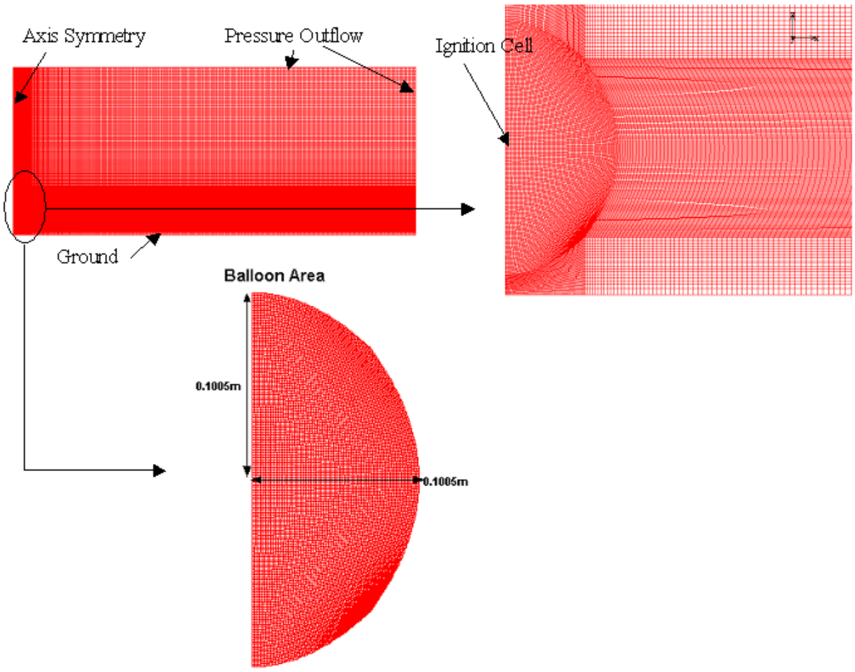

Figure 4: Computational mesh

Figures 5-8 show the temporal variation of overpressure at 1m, 2m, 5m and 18m from the center of the reactive gas cloud.

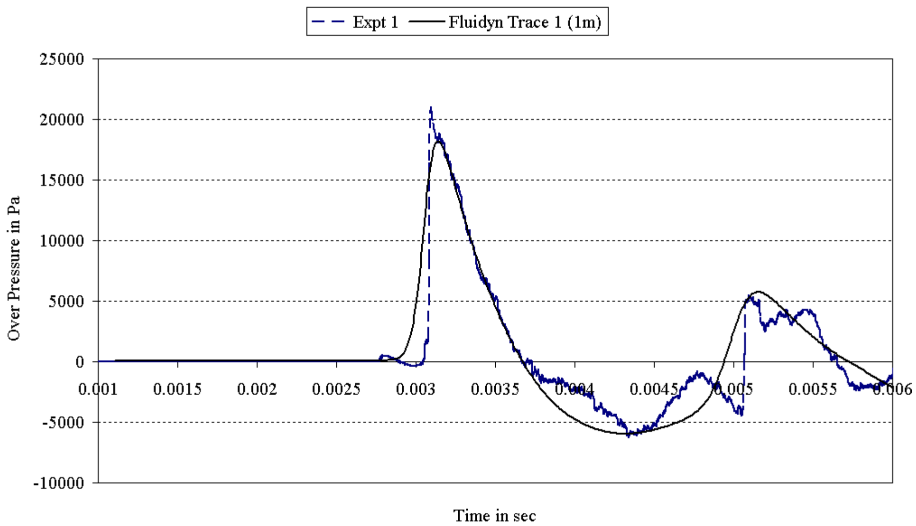

Figure 5: Overpressure variation at 1m

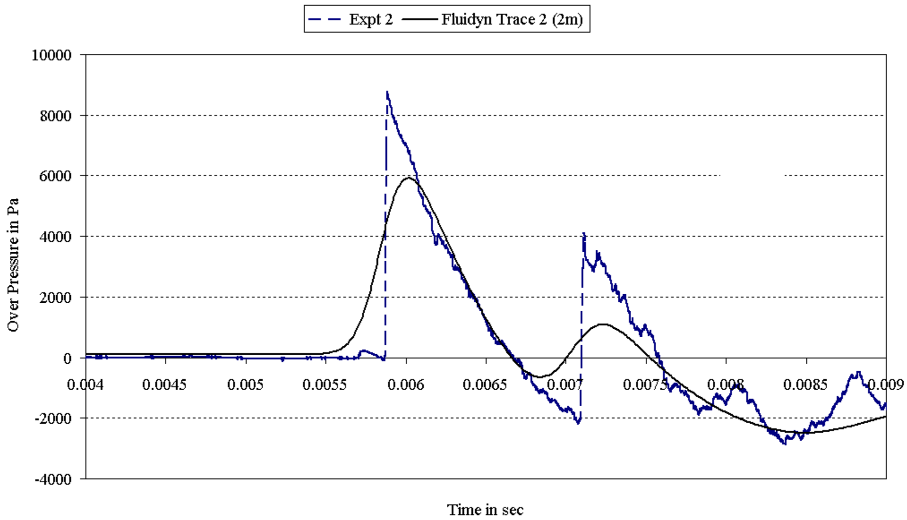

Figure 6: Overpressure variation at 2m

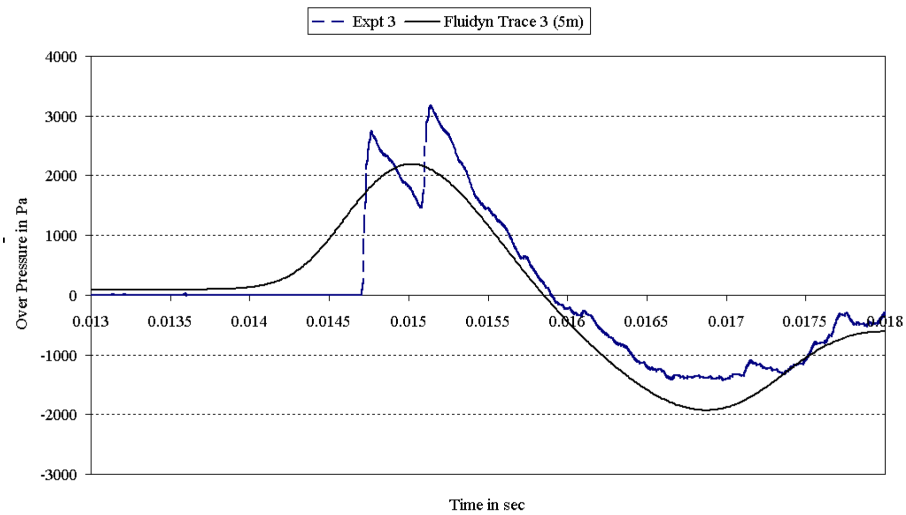

Figure 7: Overpressure variation at 5m

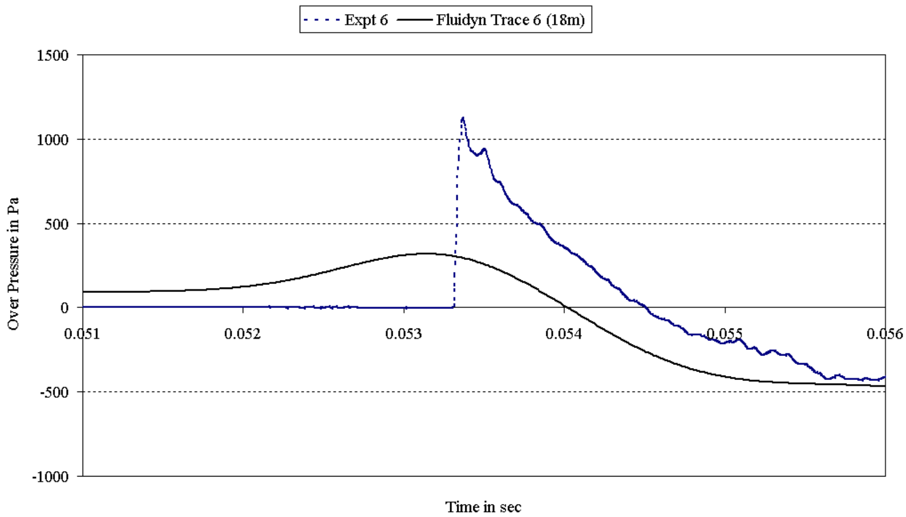

Figure 8: Overpressure variation at 18m

It can be seen that the computed overpressure history is matching very well with the experimental measurements at the first two monitor points. As the distance from the cloud increases the computed pressure wave smoothens. Also, at 5m the two distinct peaks, which are formed due to the reflection from the ground, get merged. However, the computed impulse is in good agreement with the measured value. This smoothening of the pressure wave is mainly due to the coarseness of the mesh away from the cloud and further investigations are being done with higher order numerical schemes to capture the wave more accurately for the given mesh.

4.2 Problem 2: Confined Explosion

The domain was discretized using rectangular elements with a characteristic size of 0.1 m. To get accurate results about 35200 elements had to be used. The vents were modeled using the specified pressure outflow boundary condition. A single step chemical reaction equation of the form $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ was used. The BML model was used for the flame propagation. The stretch factor was assumed to be constant and a value of 0.15 was found to be apt for comparison with the experimental measurements for the scenarios considered. Computations were performed for five different scenarios with two different reactive gas cloud volumes. All the scenarios had different vent areas. The overpressures were noted at the loaded structure as shown in Figure 2.

Table 1 compares the overpressure and the duration of explosion obtained in the present work with the experimental measurements. The difference is less than about 10 %. However, it is found that the ignition delay times observed in the simulation are less than the actual measurements. It could be because of inaccurate modeling of the ignition and this matter is being further investigated. Figures 9 and 10 show the comparison of the temporal variation of the overpressure obtained in the experiment and the present calculation for the experiments 3 and 5.

Table 1: Comparison of the computed overpressure and duration of explosion with the measurements

Exp No.	Gas Cloud length (m)	CH_4 volume fraction	Vent Area (m^2)	Max. Over Pressure (Exp) (kPa)	Time Duration (ms) (Exp)	Max. Over Pressure (Present) (kPa)	Time Duration (Present) (ms)
1	0.5	0.095	0.22	21.2	1453	23.4	1568
2	1	0.095	0.54	25.8	854	27.2	865.2
3	1	0.095	0.41	38.1	982	40.4	985.3
4	1	0.095	0.27	43.6	1045	44.9	1147
5	1	0.095	0	61.7	2693	66.0	2885.85

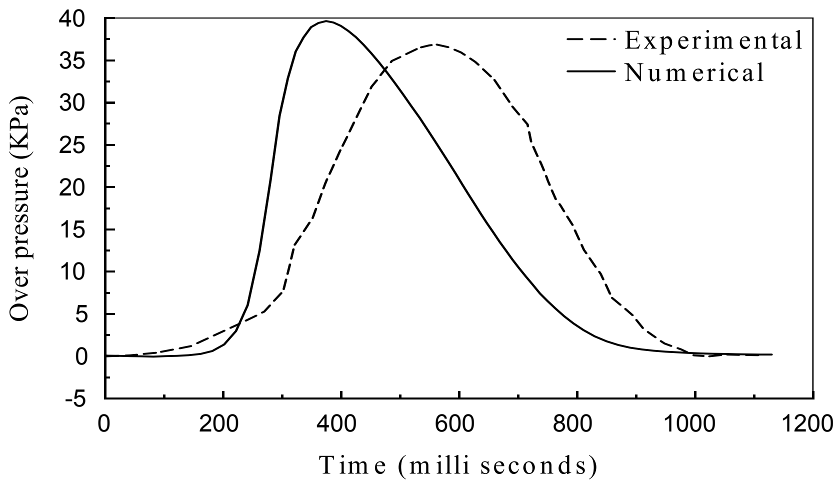

Figure 9: Variation of overpressure with time for the experiment number 3.

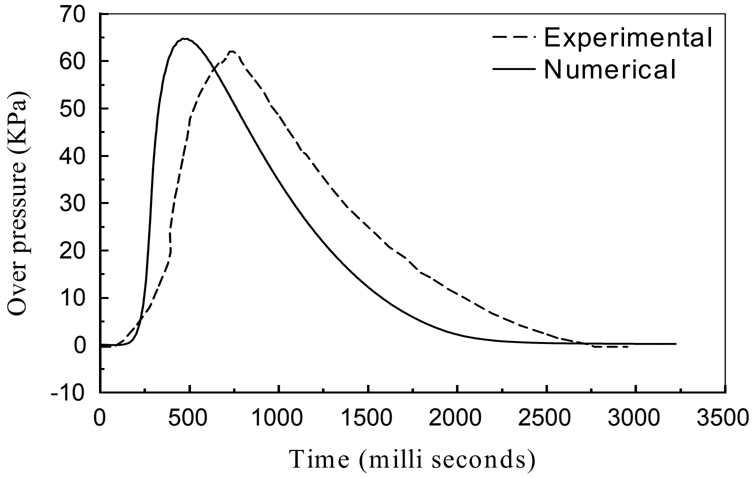

Figure 9: Variation of overpressure with time for the experiment number 5

5. CONCLUDING REMARKS

A numerical model has been developed to model the generation and dispersion of explosive gases and hazardous pollutants and possible fire and explosion due to them inside a mine environment. Various models for turbulent flows and combustion are included. Two sets of numerical studies were performed; first one concerning an unconfined detonation and the second one a confined explosion. The comparisons with the experimental measurements show good agreement. Further studies are being done with a wide range of scenarios to fine tune the explosion models to improve the accuracy and computational times.

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