# Modelling of Mitigation of Vapour Cloud Explosions Using Flame Inhibitors

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The consequences of vapour cloud explosions can be devastating causing numerous fatalities and destruction of large parts of industrial facilities. Recently a technique was suggested to mitigate vapour cloud explosions using flame inhibitors. Flame inhibitors would be injected into the vapour cloud upon gas detection. In case of ignition of the vapour cloud the flame inhibitors assure a considerable reduction of the combustion rates thus also reducing the pressures and drag loads generated by vapour cloud explosions.

Experimental results confirm the feasibility of the principle of using flame inhibitors for mitigation of vapour cloud explosions. To design systems for deployment of flame inhibitor clouds in a congested petrochemical facility assuring a considerable reduction of the explosion loads due to vapour cloud explosions it was suggested to use the dedicated CFD-model FLACS. To allow for this the combustion model was extended allowing for describing the effect of flame inhibitors on combustion and a model describing particle laden flow was implemented. The present paper presents the development of the extended combustion model and other models to represent the influence of flame inhibitors on combustion and particle laden flow, and its validation.

## 1. Introduction

Vapour cloud explosions can be devastating potentially causing fatalities and destruction of industrial plants and buildings and housing in the vicinity of the industrial facility. Recent examples include Texas City (US CSB, 2007) and Buncefield (Buncefield Major Incident Investigation Board, 2008). In spite of big progress in the field of preventive measures and methods predicting the consequences of these explosions (Hoorelbeke et al, 2006, Van den Berg et al., 2003, Plerorazlo et al. 2005) little has been done to mitigate the explosions. Water deluge activated upon gas detection has been shown to be very effective to limit consequences of explosions in congested areas offshore (Van Wingerden, 2000, Al-Hassan and Johnson, 1998) but can be difficult to apply onshore for limiting the consequences of vapour cloud explosions since large amounts of water are needed.

The feasibility of using flame inhibitors to limit the consequences of vapour cloud explosions was investigated and proven experimentally by Van Wingerden et al. (2010). The consequences of vapour cloud explosions are mainly determined by the effect congestion and partial confinement can have on flame propagation. An interaction of combustion generated flow and obstructions present in this flow establish a positive feedback mechanism causing high combustion rates and associated high static and dynamic explosion loads on equipment, structural components, buildings, etc. The flame inhibitors affect the combustion rates directly and thereby the aforementioned positive feedback mechanism.

To quantify the effects of flame inhibitors in congested petrochemical facilities and to design systems for deployment of flame inhibitor clouds in such a facility assuring a considerable reduction of the explosion loads it was suggested to use the dedicated CFD-model FLACS (Arntzen, 1998). To allow for this the combustion model was extended allowing for describing the effect of flame inhibitors on combustion and a

model describing particle laden flow was implemented. The present paper presents the development of the extended combustion model and other models to represent the influence of flame inhibitors on combustion and particle laden flow, and its validation.

## 2. Summary experimental results

Both laboratory-scale (in a 20 L vessel) and large-scale experiments (in a 50 m$^3$ congested and vented rectangular box) have been performed to investigate the possibility and feasibility for using flame inhibitors to limit the consequences of vapour cloud explosions.

The laboratory scale experiments were used to determine the effect of flame inhibitors on the laminar burning velocity for a range of hydrocarbon fuels and hydrogen varying fuel concentration. Flame inhibitor type and concentration were varied. The laminar burning velocity measurements performed on laboratory-scale revealed two main groups of flame inhibitors: those inhibiting chemically and physically (heat absorption) and those only affecting physically. Sodium bicarbonate, sodium chloride, potassium carbonate and potassium bicarbonate affect the combustion both chemically and physically. Adding relatively small amounts of these inhibitors result in a considerable decrease of the laminar burning velocity especially for leaner than stoichiometric mixtures whereas adding of calcium sulphate, manganese carbonate and magnesium carbonate only have a limited influence on the laminar burning velocity. Adding considerable amounts of the inhibitors show some effect; this most probably can be attributed to heat absorbance. The experiments further revealed that potassium carbonate can be used for vapour cloud consequence reduction in a large variety of hydrocarbons. The inhibitor however has limited effect on combustion rates in hydrogen-air mixtures.

The results of the laboratory-scale experiments have been the basis for a flame library for FLACS.

The large-scale experiments demonstrated the feasibility of using flame inhibitors to limit the consequences of vapour cloud explosions in a congested environment. Consequence reduction is possible both by injection of the flame inhibitor before and after ignition. Injection before ignition appears the most effective method. In the large-scale experiments a reduction of explosion effects by a factor of 75 has been noted (100 g/m$^3$ potassium carbonate in propane-air).

Effects seen on laboratory-scale such as the effect of flame inhibitors depending on the hydrocarbon-air mixture concentration were noted on large-scale as well. In spite of a reduced efficiency of flame inhibitors for richer than stoichiometric fuel-air mixtures still a considerable reduction of the maximum explosion overpressure in congested environments is noted over the full range of fuel-air concentrations.

The large-scale experiments demonstrated the feasibility for a number of flame inhibitors and a range of hydrocarbon substances (Van Wingerden and Hoorelbeke, 2011).

## 3. Modifications to FLACS

To be able to represent the effect of flame inhibitors some modifications were made to the FLACS code. These modifications have been described below.

### 3.1 Model for particle-laden gas

A model for particle-laden gases has been implemented based on a Eulerian mixed-fluid approach. This approach does not allow for describing deposition of flame inhibitor particles from the suspension. The mixed-fluid approach assumes that the particles and the continuous phase are in local kinetic and thermal equilibrium. This formulation affords significant computational simplicity as the initial particle size and velocity play no role in the computations and are thus not needed.

The description of particle-laden gas is based on the work of Rudinger, 1980 and implied:

- Implementation of a change of the equation of state (deviating from a perfect gas because of the use of a finite particle volume).
- A revision of the description of the internal energy and enthalpy of the equilibrium mixture.
- Implementation of the effect of presence of particles on the equilibrium speed of sound in a gas-particle mixture which can be considerably smaller than the speed of sound in the clean gas phase.

### 3.2 Release modelling

Inhibitors are released into the vapour cloud from pressurised vessels. In order to model this when designing systems for practical applications and to be able to simulate the large-scale tests described in

part 2 to validate the FLACS code the existing jet release facility in FLACS was used and adapted to describe particle-laden flow. The jet release facility has the following basis:

From a high-pressure reservoir (stagnation point), there is isentropic flow through the nozzle. This is followed by a single normal shock (where Rankine Hugoniot relations are utilized) which is subsequently followed by expansion into ambient air. No air entrainment is considered. This is based on the notional nozzle approach proposed by Birch (Birch, et al, 1984; Birch, et al., 1987). The jet release facility provides the boundary condition for the modelling of releases which has been found to give reasonably accurate results when compared to "exact" calculations.

The modifications carried out in jet release facility concern the isentropic flow equations and description of the normal shock waves (in particle laden mixture).

## 3.3 Thermodynamic and kinetic parameters for the effect of inhibitors on combustion

To model the effect of flame inhibitors on the course of explosions all relevant thermodynamic properties of flame inhibitors need to be described. The heat capacity and enthalpy data were extracted from public literature (ChemKin, 2011) and fitted in order to establish the effect of temperature on specific heat capacity and enthalpy for several inhibitors. An example is shown in Figure 1.
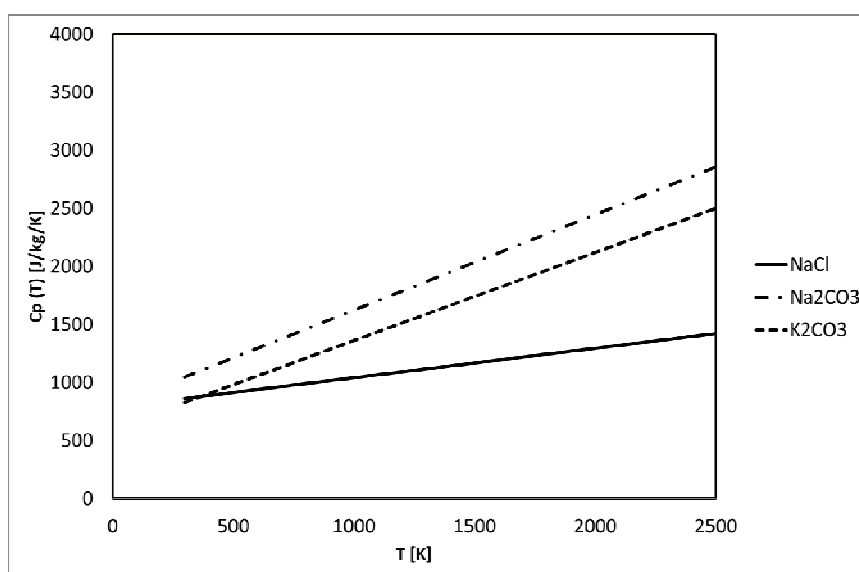


*Figure 1: Specific heat for inhibitors NaCl (table salt), $Na_2CO_3$ (sodium carbonate) and $K_2CO_3$ (potassium carbonate) as a function of temperature as implemented in FLACS.*

The experimental data from the aforementioned laboratory tests in a 20 l vessel were used to develop a flame library describing the effect of inhibitors on the laminar burning velocity: laminar burning velocity as a function of fuel concentration and inhibitor concentration for several inhibitors. Examples are given in Figure 2 showing the effect of sodium bicarbonate $NaHCO_3$ and sodium carbonate $Na_2CO_3$ on the laminar burning velocity of propane-air mixtures, respectively.
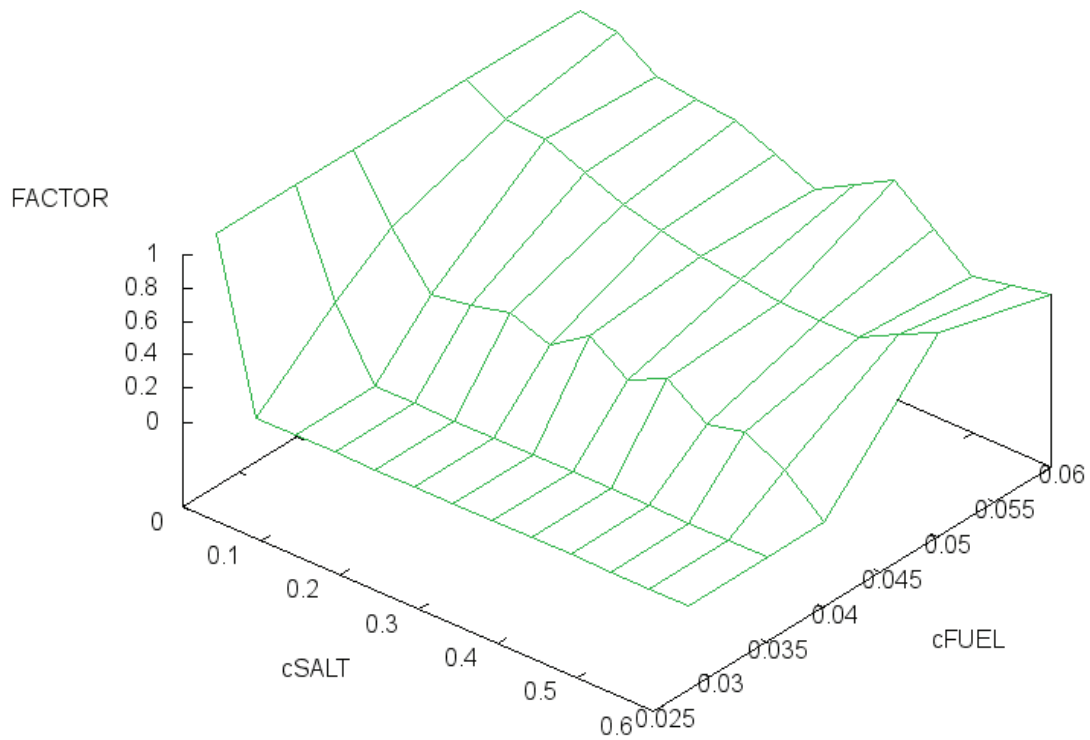
## 4. Validation

This chapter presents a comparison of simulation data compared to test results. Only a few data sets are presented here for brevity.

Figure 3 presents the simulated and observed maximum pressure obtained in a 20 L closed sphere for different concentrations of propane-air mixtures. It can be seen that the simulation results are generally within the experimental uncertainty. However, some over-prediction is seen for richer than stocihiometric concentrations (>4 %). The effect of using radiation vs. fully adiabatic simulations is also evident. The FLACS results are also seen to slightly differ from theoretical results obtained using Chemkin. This discrepancy can be explained by the fact that Chemkin uses a stirred reactor model (single control volume) while FLACS simulations involve the combustion of the reactants and their compression which implies that the temperature in the vessel is not uniform. There are also differences in the equilibrium product composition and hence the heat capacities.
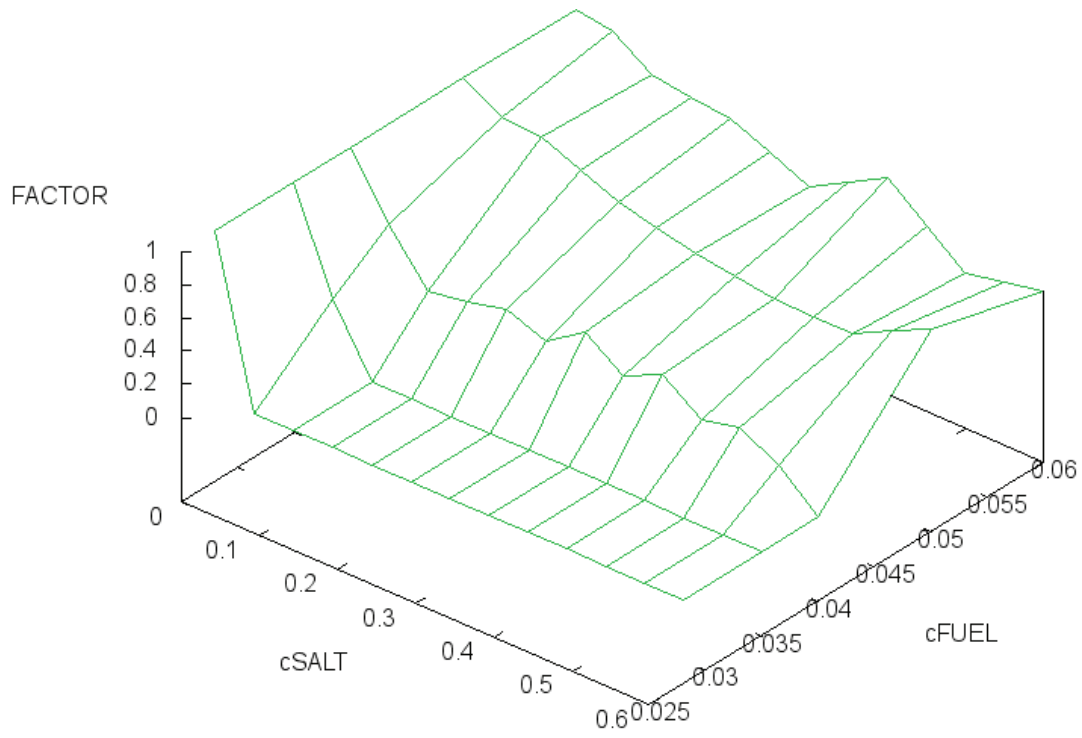
**Sodium bicarbonate (NaHCO$_3$)**



**Sodium carbonate (Na$_2$CO$_3$)**

*Figure 2: Effect of various inhibitors on laminar burning velocity of propane-air mixtures.*

## 5. Validation

This chapter gives an overview of the results of simulation of large-scale experiments performed in the 50 $m^3$ vented vessel. The results of these simulations reveal the overall quality of all implemented models. Only a few data sets are presented here for reasons of brevity.

Figure 3 presents the effect of inhibitor potassium carbonate (100 $g/m^3$) on the explosion behaviour in a 4.1 % propane-air mixture in a 50 $m^3$ vented rectangular vessel. The results of the simulations and the experiments are compared to the experimental results of a reference test (4.1 % propane-air; no inhibitor). It can be seen that the simulation of the test with inhibitor agrees reasonably well with the observed overpressure values (between 0.05-0.1 barg for both cases) but the time of arrival of the pressure peak is over-predicted significantly (0.7 vs. 0.4 s). This can be explained by the fact that the experiments involved the injection of inhibitors post-ignition implying an initial phase without the presence of inhibitors and the generation of turbulence by the injection process increasing combustion rates temporarily while the inhibitor was assumed to be present right from the beginning in the simulation affecting combustion rates immediately.
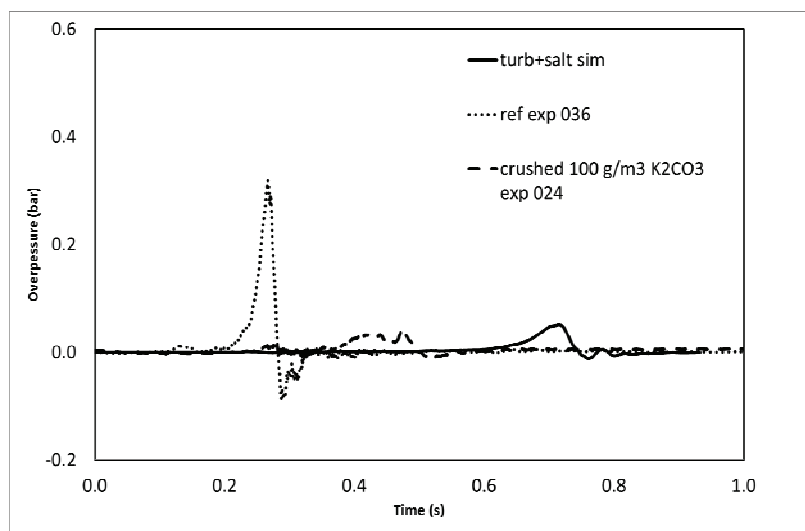


*Figure 3: Simulated and observed overpressure for explosion tests performed in a 50 $m^3$ vented rectangular vessel (4.1 % propane-air mixtures, inhibitor potassium carbonate, 100 $g/m^3$). For reasons of comparison the experimental results for a 4.1 % propane-air mixture without inhibitor is shown.*

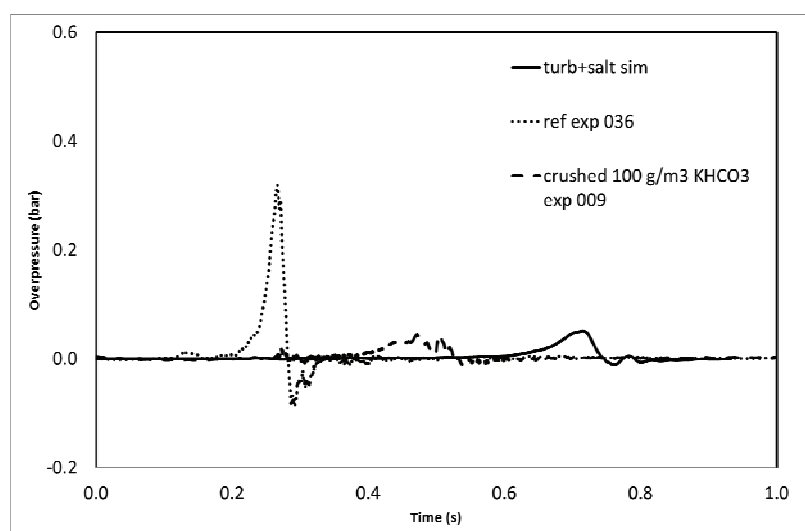Figure 4 shows similar results for potassium bicarbonate.



*Figure 4: Simulated and observed overpressure for explosion tests performed in a 50 $m^3$ vented rectangular vessel (4.1 % propane-air mixtures, inhibitor potassium bicarbonate, 100 $g/m^3$). For reasons of comparison the experimental results for a 4.1 % propane-air mixture without inhibitor is shown.*

## 6. Conclusions

Theoretical and development work has been carried out in order to extend the dedicated CFD-tool FLACS to be able to represent gas explosions in complex geometries in the presence of inhibitor salts. This has involved the implementation of new equation of state, heat capacity and enthalpy models and isentropic and normal shock equations in FLACS and the jet utility program. Certain assumptions have been made but the modelling work represents an important attempt to extend FLACS in this area.

The validation work has primarily focussed on propane-air mixtures in the presence of inhibitors and has shown that FLACS is able to represent the effect of inhibitors to a reasonable degree of accuracy.

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