Numerical study of explosion of “propylene-air” mixture cloud in recessed cavity located near complex of bluff bodies

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Abstract. The paper deals with mathematical modelling of the process of an explosion of a cloud of reactive gases and its impact on the environment. The research may be relevant to ensure fire safety and to prevent explosion hazards at industrial production facilities that use reactive gas mixtures as a working medium and at high-pressure industrial pipelines used for their transportation. The goal of the study is to develop a computational technology for numerical modelling of shock waves propagation and to predict loads on civil structures. To describe the chemical processes in the explosion, a simplified mathematical model is proposed which is based on the assumption of the infinite speed of chemical reactions. Using the model, a set of User Defined Functions is implemented in ANSYS Fluent and applied to solve a problem of a “propylene-air” cloud explosion inside the cavity located in the vicinity of two standalone buildings.

1. Introduction

The research focuses on the problem of mechanics of reactive mixture explosion. It involves complex modelling of the process that accompany technogenic explosions of clouds consisting of hydrocarbon gas mixtures. Such explosions have a highly destructive influence on industrial and urban areas.

The study may be relevant to ensure fire safety and prevent explosion hazards at industrial facilities using reactive gas mixtures as working fluids and industrial high-pressure pipelines used for their transportation.

Technogenic explosions caused by hydrocarbon gas leakages and the subsequent inflammation of hydrocarbon and air mixtures are very complex physical, chemical and mechanical processes. They involve an explosive gas leaks and formation of an explosive cloud, detonation triggering, kinetics of chemical reactions, explosion initiation, dynamics and structure of shock and detonation waves and their impact on buildings and industrial constructions.

The current research into the problem is instigated by the analysis of the disastrous explosion of propylene and air mixture happened in Kaohsiung, Taiwan in 2014. The detailed description of the catastrophe and the full analysis of the factors that premeditated it can be accessed in [1]. The
In front of the building a distance \( d = 15 \) m, a complex gas-dynamic flow is realized with transient non-homogeneous spatial distribution of pressures and temperatures. Using simplified empirical formulas allows us to describe parameters of an explosion with reasonable accuracy only in the simplest geometrical layouts [2]. Such an approach cannot be applied for modelling impacts of explosions on buildings and constructions.

Computer modelling assisted by modern engineering program complexes is a relatively universal instrument that allows predicting the impact of explosions on buildings and construction with sufficient accuracy. But applying such program complexes to solve specific practical tasks often requires developing additional modules, for instances, modules that describe kinetics of chemical reactions or heat and mass transfer processes.

To model chemical transformations, one can use a system of ordinary differential equations (ODE) that describe detailed reaction kinetic mechanisms. As a rule, a detailed kinetics of hydrocarbon oxygenation involve hundreds of reactions. Activation energies of elementary reactions can be significantly different from one another. It predetermines the stiffness of the ODE system. A solution of a multidimensional gas-dynamic problem of expansion of gas explosion products in conjunction with the stiff ODE system requires significant computing resources. An engineering method necessitates developing models that are sufficiently simplistic and do not require as much computing power as a correspondent kinetic scheme solution.

This paper focuses on the numerical research into a model problem of an explosion of a gas cloud located in a deep cavity situated in the vicinity of two buildings. To describe the chemical transformations involved in the problem, the authors developed a simplified mathematical model based on the assumption of infinite rate of chemical reactions. The model is implemented as a set of User Defined Functions (UDF) in ANSYS Fluent 19.1 and is applied to solve a problem of a gas cloud explosion in the vicinity of two standalone buildings.

2. Problem setup

As a model configuration, we consider a system of two bluff-bodies \((B1, B2)\) located on a flat plate at a distance \( d = 15 \) m from each other (Figure 1, (a), (b)). The characteristic dimensions of the bodies and the cavity are shown in Table 1. The origin of the computational domain coordinate system is located at the front wall of the second building (point \( O \) in Figure 1 (b)). The problem is solved under the assumption of symmetry with respect to the plane \( y = 0 \) m.

In front of the building \( B1 \) at a distance \( d = 15 \) m, a deep cavity of rectangular cross section is located filled with a cloud of propylene-air mixture. The initial mixture cloud is considered to be a spherical gaseous domain of \( 1 \) m radius. At the initial time moment, a cloud of propylene-air mixture explodes. The epicenter of the explosion shown in Figure 1 (a) with a red point is in the center of the cavity. The static pressure behavior is recorded in the gauges \( p1 \) and \( p3 \) installed on the frontal faces of the prisms \( B1 \) and \( B2 \) in the symmetry plane at the heights \( h/2 \) and \( h/2 \) above the ground, respectively.
Table 6. Characteristic dimensions of prisms and cavity.

| Body   | Width (along x-axis) | Height (along z-axis) | Length (along y-axis) |
|--------|----------------------|-----------------------|-----------------------|
| B1     | d = 15 m             | h₁ = 18 m             | c = 30 m              |
| B2     | d = 15 m             | h₁ = 24 m             | b = 50 m              |
| Cavity | dₑ = 4 m             | hₑ = 4 m              | c = 30 m              |

3. Mathematical model and method of computation

The calculations are performed using ANSYS Fluent 19.1 (Customer number 531496) and based on the 3D Euler equations supplemented by multicomponent gas dynamics equations and the energy equation for a mixture of gases.

To build a simplified model, we used the assumption of infinite rate of chemical reactions. At each time point, the gaseous products of the explosion are in a state of chemical equilibrium, which shifts as pressure and temperature change. As the explosion products expand and the temperature decreases, the reaction products recombine and the thermal effect of the chemical reaction increases to the maximum.

To describe the thermodynamic parameters of a chemically equilibrium gas mixture, a model [3-8] was used. The molar mass of a gas is calculated from the quadratic equation

$$\frac{\rho}{\mu} \left( 1 - \frac{\mu}{\mu_{\text{max}}} \right)^2 \exp \left( \frac{E}{RT} \right) \left( -\frac{\mu}{\mu_{\text{min}}} - 1 \right) = \frac{AT^{3/4}}{4K_v} \left( 1 - \exp \left( -\theta/T \right) \right)^{3/2},$$

whose solution is

$$\mu (\rho, T) = \frac{B \mu_{\text{min}} - 2 \mu_{\text{max}} + \left( (B \mu_{\text{min}} - 2 \mu_{\text{max}})^2 + 4(B-1)\mu_{\text{max}}^2 \right)^{1/2}}{2(B-1)},$$

where

$$B = \frac{AT^{3/4}}{4K_v} \left( 1 - e^{-\theta/T} \right)^{1/2} \cdot e^{-E/(RT)} \cdot \frac{\mu_{\text{max}}^2}{\mu_{\text{min}}},$$

The internal energy $U$ and adiabatic index of the mixture $\gamma_e$ are determined by explicit algebraic formulas:

$$U(T, \mu) = \left[ \frac{3}{4} \frac{\mu}{\mu_u} + 1 \right] + \left[ \frac{3}{2} \frac{\mu}{\mu_u} - 1 \right] \frac{\theta/T}{\exp(\theta/T) - 1} \frac{RT}{\mu} + E \left( 1 - \frac{1}{\mu_{\text{min}}} \right),$$

$$\gamma_e = 1 + \frac{R}{\mu} \left[ \frac{1 - \frac{\mu}{\mu_u}}{T} \mu_T - \frac{\rho}{\rho} \mu_p U_T - \frac{\rho}{\rho} \frac{\partial \mu}{\partial T} U_T + \mu_T \mu_p \right].$$

Algebraic formulas for derivatives $U_\mu, U_T, \mu_p, \mu_T$ are presented in [5]. The model uses the following parameters: the molar masses of the gas mixture in the atomic, extremely dissociated and...
extremely recombined states $\mu_\ell$, $\mu_{\min}$, $\mu_{\max}$, mean temperature of excitation of vibrational degrees of freedom of molecules $\theta$, average dissociation energy of reaction products $E$, generalized rate constants for the dissociation and recombination of reaction products $A$, $K_\ell$: $R$ is the universal gas constant, $T$ is the temperature. The algorithm for calculating the constants is described in [4-8]. To take into account the temperature dependence of the specific heat of the gas mixture, the UDF function DEFINE_SPECIFIC_HEAT is created using the above dependencies and integrated into ANSYS Fluent.

At the initial time moment, the computational domain is filled by the air with the following parameters: pressure $P_0 = 101.325$ kPa and temperature $T_0 = 288$ K. In the cavity, a spherical propylene-air mixture region with the center in the point (-47; 0; -2) is patched with the parameters as follows: mixture temperature $T^*=7239$ K; $P^*=9.62\cdot10^3$ kPa; the molar mass of the gas mixture $\mu^*=28.31\cdot10^{-3}$ kg/mol; $\rho^*=1.196$ kg/m$^3$. The initial static pressure field and distribution of mass fraction of the propylene-air mixture in the symmetry plane are shown in Figure 2.

![Static pressure field and mass fraction](image)

**Figure 2.** Static pressure field (a) and mass fraction of “propylene-air” mixture in the symmetry plane at the initial time $t_0=0$ ms.

Walls of the bodies, the cavity and the ground surface are modeled as non-deformable and impermeable boundaries. At the external boundaries of the computational domain the “soft” boundary conditions providing the outflow of perturbations through the boundaries were used (Figure 1, (b)).

Numerical simulation of the problem is performed using the explicit time approximation. The time step is setting during the calculation process with respect to the value of Courant number $C \approx 0.95$. Spatial approximation of the governing equations is performed using the second order upwind scheme [9]. To determine the gradients of scalar quantities, the approach based on the least square method ss used. Calculation of the fluxes at the boundaries of the grid elements is carried out using the AUSM scheme [10] that has proved itself well in calculating flows with high gradients.

The computational hexa-grid is used in the calculation. To ensure satisfied accuracy in the resolution of shocks, the grid is refined locally by embedding additional sublevels of grid cells (Cut Cells method) in the cavity and near the walls of building. The characteristic element size of the computational grid is about 2 m far from the cavity and about 0.1 m in the cavity and in zones located near the prisms. The total number of mesh elements is about $2.5\cdot10^6$.

4. **Results and analysis**

The instantaneous fields of static pressure in the symmetry plane ($y=0$) and in the $x$-$y$ cross-section ($z=0.1$ m) at several time moments are shown in Figure 3. The following main states of the flow is obtained in calculation. The primary shock wave is propagated from the epicenter of explosion in the cavity into the cavity and the surrounding space above the cavity. The results of its partial reflection from the cavity walls, formation of secondary small-scale reflected shock waves and their interaction between themselves can be seen in Figure 3 (a), (b). When expanding, the intensity of the shock is decreasing. In Figure 3(c), (d) the leading shock arrives on the frontal prism B1 and reflects from it. The interaction of the primary, reflected and secondary shock waves coming from the cavity; diffraction of the reflected primary shock wave around the first prism B1, its reflection from the plate and the second prism B2 make the whole wave pictures very complex.
Figure 3. Static pressure fields $P$ (kPa) in the symmetry plane (a, c, e, g) and in the $x$-$y$ cross-section ($z = 0.1$ m) (b, d, f, h) at the time $t = 30.3$ ms (a, b); 62.04 ms (c, d); 114.13 ms (e, f); 147.87 ms (g, h).

The cloud shape of the “propylene-air” mixture in the symmetry plane at the several time moment is presented in Figure 4. It is shown that the mixture of gases does not expand much beyond the cavity, however, the shape of the cloud changes significantly as a result of the action of reflected shock waves interfering with each other.
Figure 4. The cloud shape of the “propylene-air” mixture in the symmetry plane at the time $t = 30.3$ ms (a); 62.04 ms (c); 114.13 ms (e); 147.87 ms (g).

Figure 5 shows the static pressure history $P(t)$ at the points p1 and p3 obtained in calculations. As it is seen in Figure 5, the dynamic load on the façade of the prism B1 has several pressure peaks and several negative pressure phases. The first peak of the load with the maximum of overpressure of 6 kPa is associated with the arrival of the primary shock wave, formed during the explosion of the propylene-air mixture cloud, on the front wall of the prism B1. The secondary peaks of the load are formed due to the arrival of series of the less intense shock waves on the front wall of the prism B1 at later time points. These shocks are formed as a result of the reflection of the primary shock wave from the walls of the cavity and the multiple interference of these reflected waves. There is also a series of negative pressure phases that are long in time. These phases could be dangerous, since, from the point of view of the building safety, it could lead to the “pushing out” of building facades and window glasses into an open space in the vicinity of objects.

Figure 5. Pressure history obtained in the calculation at the gauges p1 (solid line) and p3 (dashed line).
5. Conclusions
Based on CAE ANSYS Fluent and the developed simplified mathematical model for describing the thermodynamic parameters of a chemically equilibrium gas mixture, a numerical solution is obtained for the problem of the explosion of a spherical cloud of “propylene-air” mixture in a recessed cavity near two buildings of a simple shape. According to the results of the calculations, a study is conducted of the shock-wave structure of the flow in the vicinity of buildings, and also data on the characteristic stages of dynamic loading of buildings from the spherical gas cloud explosion were obtained. Further, it is planned to refine the numerical method by introducing a detailed kinetic mechanism of the reactions in “propylene-air” mixture.

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