Propagation of shock waves formed by explosion of the air-propylene mixture in a T-pipeline

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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 and test a computational technology for numerical modelling of clouds of reactive gas mixture expansions and loads evaluation. To describe the chemical processes in the explosion, a simplified mathematical model is proposed which based on the assumption of frozen chemical reactions. Using the model, a set of User Defined Functions is implemented in ANSYS Fluent and applied for solving a problem of a “propylene-air” cloud explosion inside the T-shape tube with two closed and one open ends.

1. Introduction
Among the most important tasks of ensuring explosion safety of industrial and living environments is calculation of parameters of a blast wave generated during an explosion of a cloud of a combustible mixture in a space of complex geometry. Formation of such clouds occurs during accidental leaks of explosive liquids or gases and their mixing with air. As an example, we could refer to the disaster that took place in Kaohsiung, Taiwan in 2014 [1]. In this accident, there was leakage of liquid propylene from an underground high pressure pipeline transporting propylene from the harbour to industrial units and passing through the centre of the populous city. The vaporized hydrocarbon mixed with air and the explosive mixture cloud spread along the underground drainage system. The ensuing explosion claimed dozens of lives and led to extensive damage to residential and public buildings.

In order to describe processes of gas-air mixing and mixture ignition as well as to predict the intensity of a specific explosion and its impact on the environment, CFD simulation may be used. The paper presents the results of calculations of shock-wave flows formed as a result of an explosion in a T-shape channel with two closed ends. The calculations were carried out in the ANSYS Fluent for two
problems. First, testing of the simulation method is performed on the problem of an explosion of a spherical charge of a condensed explosive. The statement of the test problem and the initial conditions are selected in accordance with the experiment [2]. Comparisons of the results obtained using viscous and inviscid models show a good agreement with experimental data. In the second part, an air-propylene mixture cloud explosion is simulated for the same channel. The simplified simulation method is used; it is based on the hypothesis of frozen chemical reaction [3]. Under these assumptions, the gaseous products of the explosion modeled as inert mixture with the varying specific heat ratio. Based on the simulation data analysis, the structure of the unsteady process is studied, the shock wave and the hot supersonic jet coming out from the channel into open space is simulated, and the excess pressure and momentum are estimated.

2. Problem setup
The geometry under investigation is a T-shaped tube with two of its outlets closed; the third outlet is adjacent to the open space. The geometry and dimensions of the channel are shown in Fig. 1, a, where \( H=0.868 \) m, \( W=0.7 \) m, \( D=0.168 \) m, \( L1=0.360 \) m, \( L2=1.280 \) m, \( L3=1.416 \) m. Two problems are simulated for this geometry. In the first problem, the charge of a condensed explosive of a spherical shape with the mass of \( M = 185 \) g, which corresponds to a 500 kg in full scale, is placed in the tube outlet section adjoining an open air region. Figure 1 also shows the position of the three sensors P1, P2, and P3, in which the static pressure was measured in the experiment [2]. In the second problem, at the initial moment the part of the channel is occupied with a stoichiometric air-propylene mixture and the area-averaged pressure on the closed ends was monitored.

The calculations are performed in ANSYS Fluent. For the first problem several mathematical models are applied, namely inviscid gas dynamics (Model 1), Navier-Stokes equations (Model 2) and Reynolds averaged Navier-Stokes equations complemented with the \( k-\omega \) SST turbulence model (Model 3). For the second problem computations, only Model 1 is used. All models are closed with ideal gas equation of state (EoS).

The 3D calculation region, consisting of a T-shaped channel of circular cross section and an external prismatic air region, is constructed in the ANSYS Design Modeler taking into account the symmetry of the problem in the transverse direction. The origin of the global coordinate system is in the center of the sphere, which is the explosive charge. The direction of the \( x \) axis coincides with the channel axis. The calculation grids for both the problems are created in the ANSYS Meshing. The first problem grid (Fig. 1, b) is unstructured with a total cell number of approximately \( 10^6 \). It has a refinement in the charge region and includes 10 inflation layers located near the channel walls. The structured grid for the second problem (Fig. 1, c) is constructed with the sweep method and contains about \( 1.6\times10^6 \) cells. Since this problem is only computed as inviscid, no inflation layers are created.

![Figure 1. Geometry of the problem (a) and the structure of computational grids used in the first (b) and second (c) problems.](image-url)
At the boundary of the air region, pressure-outlet boundary conditions are specified. In the simulations with Model 2 and 3, adiabatic thermal conditions on the channel walls are used. At the initial time, the pipe and air space are filled with still air under normal atmospheric conditions. In the regions of condensed explosive and propylene-air mixtures, special conditions are set described in the next section.

3. Mathematical Model and Computational Method

3.1. Initial stage of condensed explosive detonation
When solving the first problem, an important issue is describing the initial stage of development of the detonation process of a condensed explosive. Various approaches are available. In ANSYS Autodyne, the behavior of condensed explosive material at high pressures and temperatures is modeled on the basis of gas dynamics equations, supplemented by the John-Wilkins-Lee EoS. Alternative methods include setting the detonation parameters at the boundary of a certain spherical region using empirical functions and the “balloon” method. In [2], it was proposed to add a source term $S$ to the energy equation that describes the energy release from the detonation as

$$ S = E_r \cdot \text{step} \left( \frac{-(t-t_0)(t-t_1)}{t_e^2} \right) $$

where $t$ is the current time [s], $t_0 = 0$ is the moment of detonation start [s], $t_1$ is the moment of detonation end [s], $t_e = 1$ s is the dimensionless parameter, $E_r$ is the energy release rate, or the explosion power [kg·m$^{-2}$·s$^{-1}$].

The values of the parameters $t_1$ and $E_r$ can be calculated on the basis of the available experimental data. The charge radius $r = 0.0141$ [m] is calculated through the volume: $V = M/\rho = 1.171 \cdot 10^3$ [m$^3$]. The energy release rate is calculated as $E_r = \Delta H \cdot M / (t_1 - t_0) = 54.351 \cdot 10^9$ [kg·m$^{-2}$·s$^{-1}$], $\Delta H$ is the specific energy; $M$ is the mass of the charge. The end of detonation is equal to the time the detonation wave travels through the charge: $t_1 = r / U = 1.65726E-06$ [s], where $U$ is the detonation velocity. Table 1 presents the parameters of the plastid explosive used in the computations.

| Table 1: Physical properties of the plastid explosive. |
|-----------------|-----------------|-----------------|-----------------|
| Parameter       | Specific energy $\Delta H$ [kJ/kg] | Density $\rho$ [kg/m$^3$] | Detonation velocity $U$ [m/s] |
| Value           | 4870            | 1580            | 8500            |

The source term works during the detonation period. As a result, high values of temperature $T = 5900$ [K], density $\rho = 1870$ [kg/m$^3$] and pressure $P = 3.1$ [GPa] are reached in the charge region.

3.2. Modeling gas cloud expansion
In the second problem, it is assumed that the explosion of the stoichiometric propylene-air mixture happens instantly. As a result, the reaction products are formed which are modeled as a special “gas” [3] with a molar weight $\mu = 28.31$ [g/mol].

Following [3], several approaches maybe used to describe the cloud expansion scenarios. The first is based on the assumption of finite rates of the chemical reactions taking place in the mixture. Depending on the composition of the mixture, a system of ordinary differential equations describing the kinetics of combustion can include hundreds of equations, which solution complicates their stiffness. The integration of such a system when solving multidimensional problems for real geometries requires significant computing time.

In addition, there are two limiting scenarios that do not require massive computations. It is assumed for both the scenarios that at the first moment in time a gas in a cloud jumps into a state of chemical equilibrium (instantaneous explosion). The first scenario assumes that all the chemical reactions are frozen, and the cloud is expanded as a chemically inert gas with a heat capacity ratio depended on temperature. The second limiting case is based on the assumption of infinite rates of the chemical
reactions. At each moment of time, the gaseous products of the explosion are in a state of chemical equilibrium, which shifts as pressure and temperature change. In this case, as the explosion products expand and the temperature decreases, the reaction products recombine and the thermal effect of the chemical reaction is maximal. Blast wave parameters calculated taking into account the detailed kinetics will fit between the corresponding parameters calculated within the framework of the limiting approximations.

A detailed description of the approaches can be found in [3]. In [4], the equilibrium approach is used to calculate the problem of the expansion of a cloud of a reacting mixture in a semi-open space. In this work, the hypothesis of “frozen” reactions is used, in which the molar composition of the mixture does not change \( \mu = \mu^* \). Internal energy \( U \), specific heats \( c_p \) and \( c_V \) and heat capacity ratio \( \gamma \) are computed by the formulas [3]:

\[
U(T) = \left[ \frac{3}{4} \left( \frac{\mu^*}{\mu_0} + 1 \right) + \frac{3}{2} \left( \frac{\mu^*}{\mu_0} - 1 \right) \frac{\theta / T}{\exp(\theta / T) - 1} \right] \frac{RT}{\mu^*},
\]

\[
\gamma(T) = \left[ \frac{3}{4} \left( \frac{\mu^*}{\mu_0} + 1 \right) + \frac{3}{2} \left( \frac{\mu^*}{\mu_0} - 1 \right) \frac{\theta / T}{\exp(\theta / T) - 1} \right] \frac{R}{\mu^*},
\]

\[
c_V = \frac{\partial U}{\partial T}_{\gamma=const} = \gamma + \frac{3}{2} \left( \frac{\mu^*}{\mu_0} - 1 \right) \frac{RT}{\mu^*} \frac{\theta / T^2}{\exp(\theta / T) - 1} \left(-1 + \frac{\theta}{T} \frac{\theta / T}{\exp(\theta / T) - 1} \right),
\]

\[
c_p = c_v + \frac{R}{\mu}, \quad H = U + \frac{RT}{\mu}
\]

where \( \mu_0 = 12.73 \) [g/mol] is a molar mass of a gas in atomic state, \( \theta \approx 2500 \) [K] is the effective temperature of excitation of vibrational degrees of freedom of molecules and \( H \) is a total enthalpy. Using these relations, a set of User Defined Functions is implemented in ANSYS Fluent and applied for solving the second problem.

Computations are performed using a density-based solver and AUSM scheme of the third order of approximation by space variables. Both implicit and explicit time-integration methods are used during one computation. For the first time period characterized by very high gradients of the flow, parameters are computed using the implicit scheme of the second order with time step of approximately 0.1 \( \mu s \) and 10 – 15 internal iteration. After 2 ms of flowtime, the pressure peaks are weakened, and since that moment the explicit time integration is used that is less computationally expensive.

4. Results and Discussions

4.1. First problem

As a result of the calculations, pressure records are obtained at the monitors \( P1 - P3 \) (see Fig. 1), as well as the fields of gas-dynamic parameters at various time moments, on the basis of which the structure of the transient flow in the channel and the shock wave output were studied and hot supersonic stream from the channel into the open space. The impact on the channel walls is due to the passage of the primary, most powerful shock wave and two waves of lower amplitude reflected from the closed ends of the channel, as well as the rarefaction wave.

In Figure 2, fields of static pressure, static temperature and Mach number fields for the first problem at the time \( t=0.5 \) ms and 1 ms computed using Model 1 are shown. At \( t=0.5 \) ms, the primary shock wave approached the region where the first pressure sensor is located. The pressure distribution shows the presence of a sufficiently extended high-pressure region with \( P_{\text{max}} = 2.23 \) MPa and a straight front, behind which a supersonic \( M = 1.6 \) flow is formed with a temperature exceeding 2200 K. A spherical shock wave (\( P_{\text{max}} = 0.4 \) MPa) first enters the free space, followed by a supersonic (\( M = 2.4 \)) hot jet (\( T = 1400 \) K).

The pressure field for time \( t=1 \) ms (Fig. 2, d) shows that the primary shock approaches the closed pipe end face and is reflected from it, resulting in the formation of a region of high pressure
(\(P_{\text{max}} = 3.8 \text{ MPa}\)) and high temperature (\(T_{\text{max}} = 2000 \text{ K}\)). The shock wave also entered the second branch of the pipe; however, the pressure and temperature parameters are much lower (\(P_{\text{max}} = 0.8 \text{ MPa}, T_{\text{max}} = 1300 \text{ K}\)).

A quantitative comparison of the data on the maximum overpressure (Table 2) and the time of arrival of the shock waves at the monitor points (Table 3) shows good agreement between the experimental data [2] and the results obtained in this work using various models. It should be noted that the most significant effect of viscosity is manifested on the secondary pressure peaks caused by the action of waves reflected from the closed channel ends. The results obtained with Models 1-3 differ by no more than 10\%, so the second problem is simulated on the basis of a more economical Model 1.

\[\text{Figure 2. Computed static pressure [Pa] (a, d), static temperature [K] (b, e) and Mach number (c, f) fields in the symmetry plane for the first problem at the time } t = 0.5 \text{ ms (a, b, c) and 1 ms (d, e, f).}\]

\[\text{Table 2. Comparison of experimental and computed overpressure values [kPa] in monitor points.}\]

| Monitor | Exp  | Model 1 | Model 2 | Model 3 | Comp [2] |
|---------|------|---------|---------|---------|---------|
| Point 1 | 1850 | 1737    | 1732    | 1686    | 2009    |
| Point 2 | 1050 | 1162    | 1064    | 1056    | 1580    |
| Point 3 | 465  | 520     | 496     | 490     | 465     |

\[\text{Table 3. Comparison of experimental and computed shock wave arrival times [ms] in monitor points.}\]

| Monitor | Exp  | Model 1 | Model 2 | Model 3 | Comp [2] |
|---------|------|---------|---------|---------|---------|
| Point 1 | 0.3  | 0.355   | 0.37    | 0.37    | 0.25    |
| Point 2 | 0.44 | 0.595   | 0.622   | 0.62    | 0.46    |
| Point 3 | 0.43 | 0.605   | 0.66    | 0.66    | 0.39    |

4.2. Second problem

At the next stage, the explosion of a cloud of air-propylene mixture in the same channel was simulated. It is supposed that the explosion of the stoichiometric propylene-air mixture \(C_3H_6 + 4.5O_2 + 16.92N_2\) happens instantly. As a result, the reaction products are formed which are modeled as a special “gas” [3] with a molar weight \(\mu^* = 28.31 \text{ [g/mol]}\) under the following conditions:
static pressure: $P^*=0.962$ [GPa] and temperature $T^*=2739$ [K]. Applying the ideal gas EoS gives the initial “gas” density value of $\rho^*=1.196$ [kg/m$^3$].

At the initial moment, the stoichiometric air-propylene mixture ("gas") occupies some part of the channel (Fig. 3, a). After the explosion causing a sharp increase in pressure, the gaseous explosion products are expanding creating a shock wave in front of them. A rarefaction wave goes inside the gas cloud. As a result, a complex gas-dynamic flow is formed with transient pressure and temperature distributions. Fig. 3 presents the dynamics of mass fraction of “gas” at various time moments. In Fig. 4, static pressure fields are shown. Fig. 5 presents the area-averaged pressure values recorded during the computations at the short (SE) and long (LE) channel ends.

![Figure 3](image)

**Figure 3.** Computed “gas” mass fraction fields in the symmetry plane for the second problem at the time $t=0$ (a), 1 (b), 4 (c), 6 (d), 8 (e) and 12 (f) ms.

5. Conclusions

In the paper, a computational technology is developed for numerical simulations of clouds of reactive mixture expansions and loads evaluation. The technology is tested on the experimental data [2]. Good agreement of experimental data and simulation result is achieved. Viscous and turbulence effects are evaluated. A simplified mathematical model is proposed to describe the chemical processes in the explosion which is based on the assumption of frozen chemical reactions. Using the model, a set of User Defined Functions is implemented in ANSYS Fluent and used to simulate a problem of a propylene-air cloud explosion inside a T-shape tube with one open and two closed ends. Based on the data analysis, the structure of the unsteady flow in the channel, the exit of the shock wave (SW) and the hot supersonic jet from the channel into the open space were studied, and the excess pressure and impulses were estimated.
Figure 4. Computed static pressure fields in the symmetry plane for the second problem at the time $t=1$ (a), 2.5 (b) and 6 (c) ms.

Figure 5. Computed area-averaged static pressure history recorded at the short (SE) and long (LE) closed channel ends.

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