



# A 3D numerical study on the effects of obstacles on flame propagation in a cylindrical explosion vessel connected to a vented tube



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## ABSTRACT

This article presents a numerical study of the explosive wave propagations from a 40 cm long and 10.8 cm diameter cylinder to smaller 1.7 m and 2.6 m long cylinders with 36 mm diameters. Initially, the 40 cm long cylinder was filled with 4% propane-air mixtures and ignited with a 1 kJ sparking energy until the maximum temperature near the ignition source reached 2400/3000 K. In the study, a 3D numerical model was established by combining compressible four-step reduced propane oxidation reaction kinetics with the  $k-\omega$  shear-stress transport (SST) turbulent model. In order to resolve the thin detonation wave front, a dynamically refined mesh near the high pressure gradient was adopted. The pressure gradient profiles, velocity magnitude contours, temperature contours and compressible wave propagation speeds across the tubes were then predicted using this 3D model.

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## 1. Introduction

There are several studies on gas and dust explosions originating in a vessel and discharged through a relief tube, such as Du et al. (2014), Kersten and Forster (2004), Kindracki et al. (2007), Lunn et al. (1988), Ma et al. (2015), Na'inna et al. (2013), Seiler et al. (2006), Ural (1993), Zhang et al. (2013), Zhou et al. (2012) and Zipf et al. (2013). Relief ducts are especially required when the expulsion of hot, and sometimes toxic, gases flowing violently out from the vent and the gaseous stream has to be avoided in the area close to the vessel, especially inside buildings. Since the 1980s, it has been well known that the addition of a duct to a vessel results in a pressure hike following an explosion which may impede the venting effect. Ponizy et al. (2014a) suggested that the pressure hike in the vessel connected to a vented tube is caused by a secondary explosion ("burn-up") occurring in the duct.

Molkov et al. (1984) designed an experiment with a vessel connected through a duct. He observed that shortly after the flame entered the duct, the pressure in the duct exceeded the pressure in the vessel for several milliseconds, and a fast backward flow was established which disrupted the flame front in the vessel, accelerating the combustion process and generating a considerable

increase in the maximum vessel pressure. Ponizy and Leyer (1999a) presented an exhaustive experimental study of the phenomenon in a laboratory-scale vessel connected to ducts of different lengths and diameters, and discussed the influence of vessel-duct interaction on flame dynamics. Ponizy and Leyer (1999a,b) found that secondary explosions (also called burn-up and explosion-like combustion) initiated in the duct played a more important role in the increase of the explosion overpressure than other factors. Henneton et al. (2006) visualized the secondary explosion phenomenon in a duct for gas explosions by using a cylindrical Plexiglas transparent vessel-duct arrangement, and a high frame rate video camera. Yan et al. (2014) used a 20 L spherical chamber at elevated static activation overpressures, ranging from 1.8 bar to 6 bar, with duct diameters of 15 mm and 28 mm, and duct lengths of 0 m (simply venting), 1 m and 2 m. They also monitored explosion pressures, both in the vessel and in the duct, by pressure sensors with a frequency of 5 kHz. They observed that the secondary explosion occurring in the duct increases the maximum reduced overpressure in the vessel.

There are a number of publications using a two/three-dimensional computational fluid dynamics CFD tool to predict some of the explosion characteristics of an explosion vessel connected to a relief tube. Ferrara et al. (2006) modelled gas explosions vented through ducts by using a two-dimensional (2D) axisymmetric CFD model based on the unsteady Reynolds Averaged Navier Stokes (RANS) approach, in which the laminar, flamelet and

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distributed combustion models were implemented. They observed that after the flame enters the duct, a sharp increase in the duct pressure occurs, inducing a temporary sign reversal of the pressure difference across the duct entrance, leading to an effective flow reversal. They defined the reversed flow as “burn up”. However, this model did not reveal the temperature distribution before and after the flame entering the connected tube from the vessel, thus not verifying the secondary explosion theory of Ponizy et al. (2014b). Ponizy et al. (2014b) also used two-dimensional axisymmetric grid of about 60,000 quadrilateral cells of the same height (0.5 mm) and different lengths (from 4 mm to 0.5 mm) to predict the flowing properties of the 40 cm long and 10 cm ID vessel connected with 16/21/36 mm ID 2.6 m tubes filled with stoichiometric propane-air mixtures, showing that the secondary explosion in the duct (“burn-up”) has its origin in a turbulent zone, appearing at the duct entrance at the moment of the flame passage. However, the 2D models cannot simulate the effects of obstacles on the flame propagation speeds because obstacles will invalidate the axisymmetric assumptions.

There are some reports on the study of the effects of obstacles in the explosion vessel or the connected tubes on the maximum pressure or maximum rate of the pressure rise. Zhou et al. (2012) studied the effects of the ignition location, shapes of the obstacles and distances between the obstacles on the maximum pressure and maximum rate of the pressure rise using a methane-coal dust hybrid system in a closed tube. They observed that hollow obstacles linked with the inner wall of the tube induced faster pressure rising than where centre blocked solid obstacles were installed, and obstacles with more sharp corners induce more violent explosions, with the most dangerous explosion occurring when the spacing between the obstacles almost equalled the inner diameter of the tube for the same size obstacle. Kindracki et al. (2007) examined the influence of the ignition position and obstacles on the explosion development in premixed methane–air mixtures in an elongated explosion vessel with 1325 mm length tube with 128.5 mm diameter and two grids of steel block. They concluded that the flame propagation and pressure variation in the long tubes with/without obstacles are very sensitive to the location of the ignition point and the size and the shape of the obstacles. Na'inna et al. (2013) used a vented cylindrical vessel 162 mm in diameter and 4.5 m long to study the effects of the separation distances of two low blockage (30%) obstacles. They showed that the worst case separation distance for a low blockage double obstacle was 1.75 m, which produced close to 3 bar overpressure and a flame speed of about 500 m/s, which were of the order of twice the overpressure and flame speed with a double obstacle separated 2.75 m apart. There are few reports on the effects of obstacles in an explosive vessel connected with a vented tube on the characteristics of the flame propagation.

The present study will focus on revealing numerically the characteristics of the flame propagation from an explosive vessel with obstacles to a vented tube. The effects of the turbulence of the vented tube diameter, due to the introduction of obstructions in the explosive vessel, on the flame speed will be studied. The details of the flame entering into the vented tube from the explosive vessel will be revealed by snapshot animations or the contours of temperature, velocity and molar fraction of the fuel.

## 2. Mathematical expressions and computational domains

### 2.1. $k$ - $\omega$ Shear-stress transport (SST) turbulent model

The following governing equations are included in this paper for completeness. For details, refer to the theoretical guide from Ansys Fluent 15.1 (2015). The two-equation  $k$ - $\omega$  shear-stress transport

model (written in conservation form) is given by the following (Menter, 1994):

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = P - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right] \quad (1)$$

$$\begin{aligned} \frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = & \frac{\gamma}{\nu_t} P - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j} \right] \\ & + 2(1 - F_1) \frac{\rho \sigma_{\omega 2}}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \end{aligned} \quad (2)$$

In which

$$P = \tau_{ij} \frac{\partial u_i}{\partial x_j} \quad (3)$$

$$\tau_{ij} = \mu_t \left( 2S_{ij} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \rho k \delta_{ij} \quad (4)$$

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (5)$$

and the turbulent eddy viscosity is computed from:

$$\mu_t = \frac{\rho a_1 k}{\max(a_1 \omega, Q F_2)} \quad (6)$$

Each of the constants is a blend of an inner (1) and outer (2) constant, blended via:

$$\phi = F_1 \phi_1 + (1 - F_1) \phi_2 \quad (7)$$

Where  $\phi_1$  represents constant 1 and  $\phi_2$  represents constant 2. Additional functions are given by:

$$F_1 = \tanh(\arg_1^4) \quad (8)$$

$$\arg_1 = \min \left[ \max \left( \frac{\sqrt{k}}{\beta^* \omega d}, \frac{500 \nu}{d^2 \omega} \right), \frac{4 \rho \sigma_{\omega 2} k}{CD_{k\omega}} \right] \quad (9)$$

$$CD_{k\omega} = \max \left( 2 \rho \sigma_{\omega 2} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 10^{-20} \right) \quad (10)$$

$$F_2 = \tanh(\arg_2^2) \quad (11)$$

$$\arg_2 = \max \left( 2 \frac{\sqrt{k}}{\beta^* \omega d}, \frac{500 \nu}{d^2 \omega} \right) \quad (12)$$

where  $\rho$  is the density,  $\nu_t$  is the turbulent kinematic viscosity,  $\mu$  is the molecular dynamic viscosity,  $d$  is the distance from the field point to the nearest wall, and  $\Omega = \sqrt{2W_{ij}W_{ij}}$  is the vorticity magnitude, with

$$W_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) \quad (13)$$

The constants are:

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