Numerical Investigation of Constant Volume Propane-Air Explosions in a 3.6-Metre Flame Acceleration Tube

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1 Introduction

Fuel-air explosions represent a severe hazard in industry. The chain of events for a typical vapour cloud explosion entails loss of containment of gaseous and/or liquid fuel, evaporation (liquids), dispersion and mixing, ignition of the flammable cloud, turbulent premixed combustion and pressure build-up, and propagation of blast waves in the surroundings. The primary mechanism for flame acceleration in highly congested geometries is the positive feedback between expansion of combustion products, generation of turbulence in the unreacted mixture, especially in wakes behind obstacles, and enhanced rate of turbulent combustion [1]. Safe design of industrial facilities and optimal implementation of risk-reducing measures require models that can estimate the consequences of explosions with sufficient accuracy. Computational fluid dynamics (CFD) represents the current state-of-the-art in engineering models for assessing the consequences of gas explosions in complex geometries. In the context of simulating industrial accident scenarios as part of quantitative risk analyses, most commercial CFD tools rely on turbulence models based on the Reynolds-averaged Navier-Stokes (RANS) equations, such as the k-ε model [2]. A special class of CFD codes have adopted the porosity/distributed resistance (PDR) concept for representing relatively small geometry objects on a coarse computational mesh [3-7].

The combustion model in the CFD/PDR tool FLACS includes an empirical correlations for the turbulent burning velocity S_T in flammable mixtures [7-9]. Recent experiments indicate that the current model system under-predicts the rate of combustion in fuel-rich propane-air mixtures [9-10]. The purpose of the work presented here is to explore an alternative correlation for S_T [11], which incorporates the effect of the strain rate Markstein number Ma_{sr} on the turbulent burning velocity. Results from experiments in a 3.6-m flame acceleration tube [9-10] are compared with predictions from CFD simulations with two different correlations for turbulent burning velocity, over a wide range of fuel concentrations.

2 Model system

The numerical solver Flacs in the CFD tool FLACS is a three-dimensional CFD code that solves Favre-averaged transport equations for mass, momentum, enthalpy, turbulent kinetic energy (k), rate of dissipation of turbulent kinetic energy (ε), mass-fraction of fuel and mixture-fraction on a structured Cartesian grid using a finite volume method [12]. The RANS equations are closed by invoking the ideal gas equation of state and the standard k-ε model for turbulence [2]. Flacs solves for the velocity components on a staggered grid, and for scalar variables, such as density, pressure and temperature, on a cell-centred grid. The accuracy of the Flacs solver is second order in space and first/second order in time. FLACS uses the SIMPLE pressure correction scheme [13], extended with source terms for the compression work in the enthalpy equation, for compressible flows, and the SIMPLEC scheme for non-compressible flows.

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The purpose of a combustion model for premixed combustion is twofold: to define the reaction zone (i.e. the position of the flame), and to specify the rate of conversion from reactants to products (i.e. the rate of energy release). The default flame model in FLACS is the so-called β model [14], where flame thickness is constant, typically about three grid cells, and the flame propagates with a specified burning velocity defined by an empirical burning velocity model. The model originates from theory for flame stretch and experimental results for gaseous flames [15-16]. Abdel-Gayed *et al.* [15] used dimensionless parameters to correlate 1650 separate measurements of turbulent burning velocity for premixed gaseous mixtures, and Bray [17] expressed the data from Abdel-Gayed by the empirical expression:

$$\frac{S_T}{S_L} = 0.875\, K^{-\varphi}\, \frac{u'_{rms}}{S_L} \tag{1}$$

where K is the Karlovitz stretch factor, u'_{rms} is the root-mean-square of the turbulent velocity fluctuations, and S_L is the laminar burning velocity. Eq. (1) is valid for Lewis numbers $Le \leq 1.3$. Under certain assumptions [10, 14], and for the original value of the constant φ (= 0.392), the turbulent burning velocity can be expressed as:

$$S_T = 1.81 \cdot S_L^{0.784}\, u'^{\,0.412}_{rms}\, \ell_I^{0.196}\, \nu^{-0.196} \approx 15.1 \cdot S_L^{0.784}\, u'^{\,0.412}_{rms}\, \ell_I^{0.196} \tag{2}$$

where ℓ_I is the turbulence integral length scale. The latter expression in Eq. (2) assumes a kinematic viscosity υ equal to 0.00002 m^2 s^{-1}.

The laminar burning velocity is the only parameter in Eq. (2) that represents the reactivity of the mixture. However, results from explosion experiments with propane-air mixtures in a closed 20-litre vessel, over a wide range of concentrations and turbulent flow conditions [18], suggest that Eq. (2) cannot be valid over the entire flammable concentration range. Validation against explosion experiments performed in a 3.6-m flame acceleration tube show that FLACS under-predicts the rate of combustion for fuel-rich propane-air mixtures [9-10]. The approach adopted for improving the predictive capabilities in FLACS for fuel-rich propane-air mixtures is to implement an alternative correlation that incorporates fuel specific effects on S_L arising from sensitivity to flame stretch. Bradley and co-workers [11] proposed a correlation based on the strain rate Markstein number Ma_{sr} that will be used in the present study:

$$S_T = \alpha K^{\beta} u'_k \quad \text{where} \begin{cases} \alpha = 0.023\left(30 - Ma_{sr}\right) \text{ and } \beta = 0.0103\left(Ma_{sr} - 30\right) & \text{for } Ma_{sr} > 0 \\ \alpha = 0.085\left(7 - Ma_{sr}\right) \text{ and } \beta = -0.0075\left(Ma_{sr} + 30\right) & \text{for } Ma_{sr} < 0 \end{cases} \tag{3}$$

Eq. (3) is valid for $K > 0.05$. In the present study, results obtained with the standard version of FLACS, using Eq. (2), will be compared with results obtained with a special version that incorporates Eq. (3).

Due to the relatively large aspect ratio of the vessel (L/D>13), and the limited spatial scale of the experiments, the CFD simulations must account for the effect of radiative heat transfer from the hot combustion products to the walls of the vessel. Hence, all simulations included a 6-flux model based on the composite-flux approach. The model solves the radiative transfer equation approximately via six first-order differential equations, corresponding to the positive and negative radiation fluxes in the three coordinate directions [19]. The present study is limited to 3.0 cm cubical grid cells throughout the computational domain, since further refinement would be in violation with stated grid guidelines [12].

3 Experiments

Figures 1 and 2 show the 3.6-m flame acceleration tube. The main apparatus consists of three 1.2-m sections with internal dimensions 0.27 m × 0.27 m, connected by flanges. Each section is fitted with a separate dispersion system, pressure transducers (P1-P3), flame probes (T1-T3), windows for visual flame tracking, and brackets for fixing additional obstacles [9-10]. The dispersion nozzles, brackets and probes represent inherent obstacles (Figure 1, right). Table 1 summarizes the experiments.

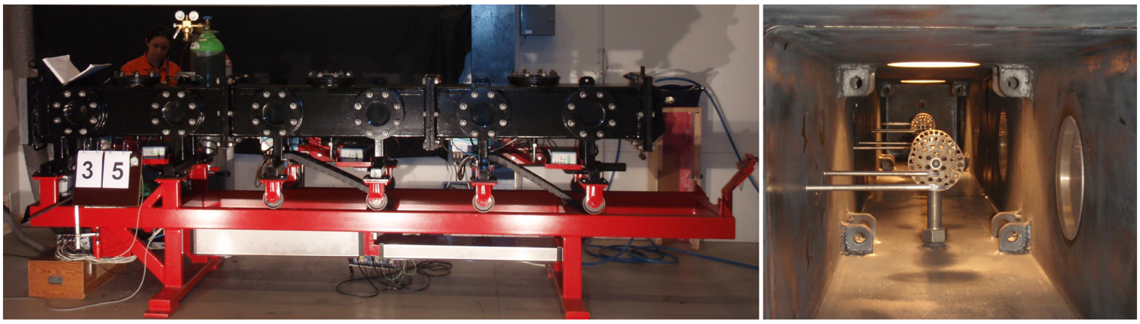

Figure 1. The 3.6-m flame acceleration tube (left) and internal geometry (right).

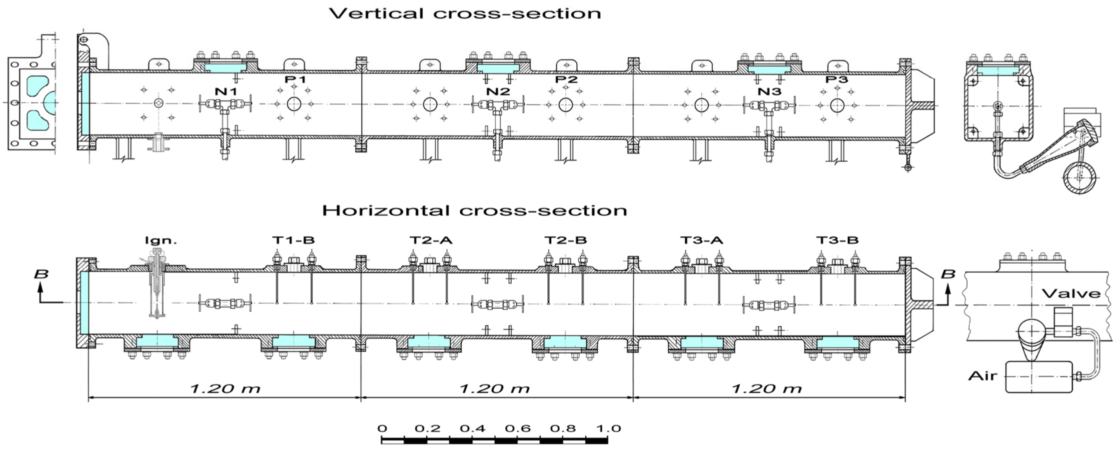

Figure 2. Schematic of the 3.6-m flame acceleration tube.

Table 1: Summary of test conditions, test numbers and maximum explosion pressures.

Initial conditions	**Test no.**		**Concentration**	**Explosion pressure** (bar*g*)	
Propane Initially quiescent Spark ignition	18	26	3.0 vol.% (ER 0.73)	3.9	3.8
	20	28	4.5 vol.% (ER 1.12)	6.8	6.7
	22	30	6.0 vol.% (ER 1.52)	5.8	5.6
	24	32	7.5 vol.% (ER 1.93)	2.8	2.8
Propane Initially turbulent: t_v = 1.0 s Spark ignition	7	13	3.0 vol.% (ER 0.73)	5.2	4.6
	8	14	4.5 vol.% (ER 1.12)	6.9	7.0
	9	15	6.0 vol.% (ER 1.52)	6.3	6.2
	10	16	7.5 vol.% (ER 1.93)	3.9	4.5

Piezoelectric pressure transducers (Kistler 701A) and charge amplifiers (Kistler 5011) measured the pressure development in the tube. Flame propagation along the tube was recorded with a digital high-speed video camera (Phantom v210), and measured with ten 0.3 mm type K thermocouples, mounted on rods to reach the centre-line of the tube. In all tests, a vacuum pump was used to evacuate the vessel, and the pressure was adjusted to 0.60 bar*a* prior to injection of air from three pressurized (17.2 bar*a*) reservoirs of volume 2.0 litre each. The amount of propane added to the vessel was controlled by monitoring the pressure. For tests under initially turbulent conditions, the ignition source is triggered 1.0 s after onset of dispersion. Testing of propane under initially quiescent conditions follow the same procedure, but with ignition triggered several minutes after completing the injection process. Figure 2 shows the position of the spark gap (ignition source). Further details are described elsewhere [9-10].

4 Results and discussion

Figures 3-5 summarize experimental and simulated results for propane-air mixtures ignited by spark discharges under initially quiescent conditions. The results include three pressure measurements from each experiment and each simulation, the mean pressures (thick lines), and flame arrival times at the various sensors (data points marked on the pressure-time curves).

For the lean mixture (3.0 vol.%), the maximum pressure occurs before the flame front reaches the end of the tube. This demonstrates the strong effect of heat losses for this type of systems. In general, the simulations over-predict the rate of combustion, especially during the initial phase of flame propagation. The results obtained with Eq. (2), marked 'Sim. Std.', and with Eq. (3), marked 'Sim. Ma.', do not differ significantly for near stoichiometric mixtures, but there are clear signs of improvement for both the lean and the rich mixtures. Ignition of the very rich mixtures (7.5 vol.%) in tests 24 and 32 (Table 1) resulted in a barely visible flame propagating upwards from the point of ignition, and continuing along the upper part of the tube. This scenario was not simulated with FLACS.

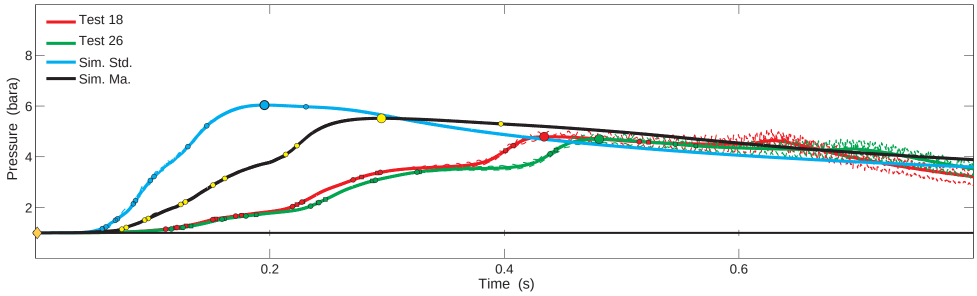

Figure 3. Results for initially *quiescent* mixtures of 3.0 vol.% propane in air (ER 0.73).

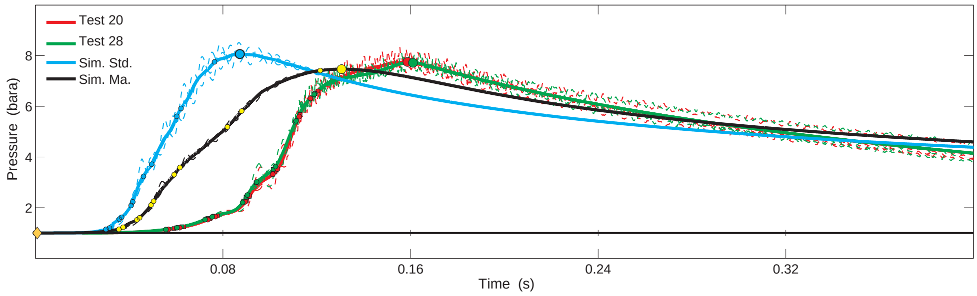

Figure 4. Results for initially *quiescent* mixtures of 4.5 vol.% propane in air (ER 1.12).

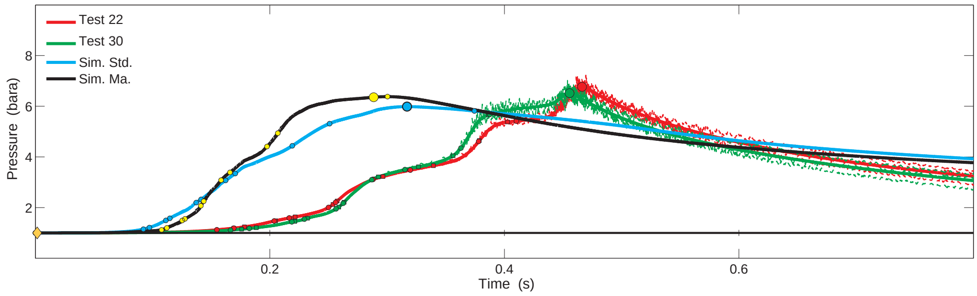

Figure 5. Results for initially *quiescent* mixtures of 6.0 vol.% propane in air (ER 1.52).

Figures 6-9 summarizes the results for propane air mixtures ignited by spark discharges under initially turbulent conditions. It is evident that the effect of the initial turbulence is significant, especially for the fuel-rich mixtures. The simulations with the default model (2) over-predict the rate of combustion for the lean and stoichiometric mixtures, and under-predicts for the very rich mixture. The new model represents a significant improvement for all mixtures except from 6.0 vol.% propane in air.

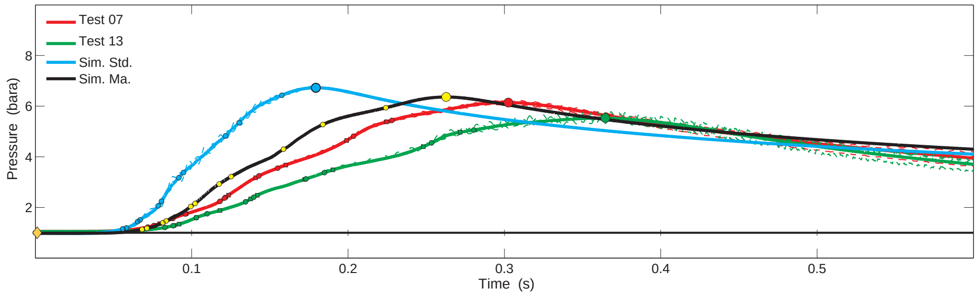

Figure 6. Results for initially *turbulent* mixtures of 3.0 vol.% propane in air (ER 0.73).

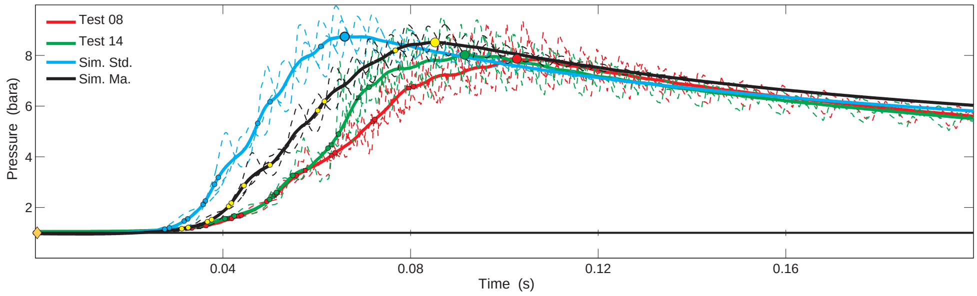

Figure 7. Results for initially *turbulent* mixtures of 4.5 vol.% propane in air (ER 1.12).

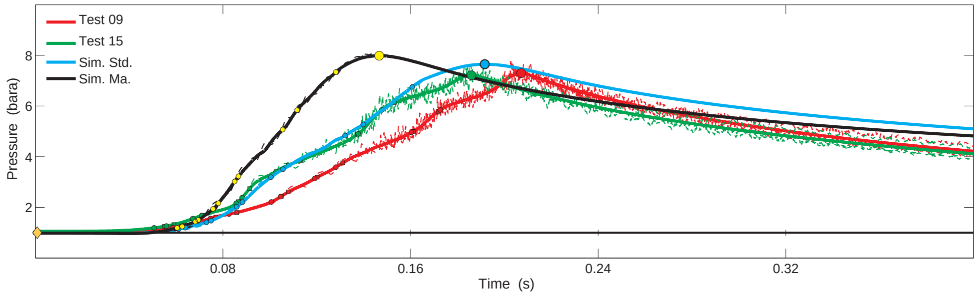

Figure 8. Results for initially *turbulent* mixtures of 6.0 vol.% propane in air (ER 1.52).

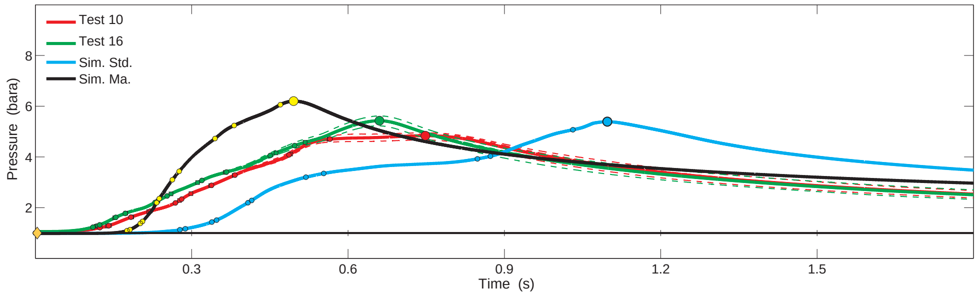

Figure 9. Results for initially *turbulent* mixtures of 7.5 vol.% propane in air (ER 1.93).

6 Conclusions and suggestions for further work

The results obtained with the correlation for turbulent burning velocity that incorporates the effect of the strain rate Markstein number [11] represent a significant improvement for both lean and very rich propane-air mixtures, relative to the standard correlation [17]. Although the results are encouraging, further validation and model improvements are necessary. It is not straightforward to obtain reliable values for S_L and Ma_{sr} for the fuel-rich mixtures, and the model system is sensitive to both parameters. Future work will include validation against experiments in larger geometries and for various fuels. Given the relatively complex internal geometry of the 3.6-m flame acceleration tube, it is necessary to consider the effect of the sub-grid models for initial flame propagation and turbulence production.

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