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Comparison of Explosion Methods for Large-Scale Unconfined Elongated Explosions with Propane and Methane mixtures

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Abstract

Existing methods for flame propagation and deflagration to detonation transition (DDT) prediction can be divided into three main categories: empirical models, phenomenological and Computational Fluid Dynamics (CFD) based. The former relies on correlations derived from experimental tests and are usually very simple and fast to apply. Phenomenological methods are simplified models which represent the major physical processes in the explosion. CFD-based models, on the other hand, are more sophisticated and require a high degree of expertise for its usage and data analysis. Although all three types of methods are extremely useful for overpressure and flame speed prediction in scenarios involving accidental industrial explosions, they usually fail to predict the occurrence of deflagration-to-detonation transition (DDT) and flame acceleration for low and medium reactivity fuels, such as propane and methane, in elongated clouds. This can be related to the fact that detonation onset or highly turbulent flames are often ignored for such types of fuel. Having that in mind, this paper aims to conduct a review of current explosion models and compare them to recent large-scale tests with premixed propane-air and methane-air mixtures. The ultimate goal is to identify main flame parameters to be included in explosion analysis and propose modifications to improve overpressure and flame speed prediction for elongated vapor clouds.

Keywords: VCE, deflagration-to-detonation transition, explosion safety

1 Introduction

Flame propagation and explosion behavior of hydrogen and hydrocarbon-based mixtures remain critical issues for explosion safety in chemical plants, refineries, and nuclear power plants. In the last decades, a considerable number of incidents related to accidental releases of large quantities of flammable mixtures followed by ignition has been observed [1]. One of the most notorious cases include the explosions inside an oil terminal in Jaipur, India (October 2009) [1]. A gasoline leak that lasted around 75 minutes before ignition, resulted in a vapor cloud explosion that led to eleven deaths and several tank fires. Damage reached a distance of 2 kilometers. Evidence led to the conclusion that transition to detonation was the only possible explosion mechanism. In another instance, the explosion in Buncefield fuel storage depot in December 2005 measured 2.2 on the Richter scale and caused immense destruction to the area around, the damage reaching a radius of 1.5 kilometers, whereas the explosion was confined in a small area [2].The severity of the explosion could not have been predicted by any major hazard assessment method of the time [2].

Such incidents highlight the importance of proper design and robustness of explosion mitigation methods. From the practical point of view, safety professionals work towards estimating flame speeds and maximum overpressure build-up for a wide range of industrial releases scenario. This information is used to support safety design decisions and protective measure specifications. Defining the entire spectrum of plausible scenarios is not a straightforward task, it must address all affecting parameters including release locations, mixture concentration, the volume of flammable cloud, equipment density and disposition, and ignition position. This problem can be simplified by identifying and ranking conditions that are likely to lead to more severe explosion cases. Therefore, researchers have proposed empirical correlations [3]and numerical codes [4][to account for obstruction characteristics (equipment density and spacing) that might lead to deflagration to detonation transition (DDT) during explosion modeling analysis.

Existing methods for flame propagation and DDT prediction can be broadly divided into three categories: empirical models, phenomenological methods, and computational fluid dynamics (CFD) codes [1]. Empirical models are based on correlations derived from experimental results and are usually very simple and fast to apply. The Baker-Strehlow-Tang (BST) curves are an example of such a model that has been used extensively by oil and gas industry. They were updated in 2005 to include the likelihood of DDT and estimate overpressure based on flame speed [2]. This flame speed depends on three parameters: reactivity, confinement and congestion. There have been several efforts to improve the model by redefining the parameters and incorporating ground effects [3]. Another example is the TNO multi-energy method which predicts the overpressure based on strength curves [4].

CFD codes, on the other hand, tend to be more time consuming and require a certain degree of expertise to interpret the results. Models of this type calculate the overpressure by solving the Navier-Stokes equations and include additional sub-models to incorporate the effect of turbulence and combustion [5]. FLACS™ is one of the commercially available CFD package and has a specific methodology to predict the potential of DDT. This method has been validated against several small-scale experiments involving different types of fuel [6].

The primary goal of this study is to conduct a review of current explosion models and understand their limitations. The objective is to compare predicted results against recent large-scale tests with premixed propane-air and methane-air mixtures for elongated clouds [refer gexcon report].

2 Current explosion models used for comparison

An initial screening of the current methods utilized for large scale explosion modelling was made. A summary of the most common methods used can be seen in **Error! Reference source not**

found. grouped by their model type. Some methods were later discarded from this analysis due to the lack of guidance available in the open literature.

Table 1. List of common explosion methods for overpressure and flame speed prediction

Type of Model	List of Models Considered Initially	Source
Phenomenological	CLICHE*	[5]
	SCOPE*	[6]
Empirical Correlations	TNT Equivalent Method	[7, 8]
	TNO Multi-energy Method (MEM)	[9-11]
	BST	[3]
	Primary Explosion Site (PES)	[12-14]
	CAM Method Version 2	[15, 16]
	Melton and Marx correlation for flame speed	[17]
	Li *et al* (2014) Correlation	[18]
	Elongated VCE Blast Waves (Baker Risk)*	[19]
Numerical Models	REAGAS *	[20]
	EXSIM*	[21]
	FLACS*	[4]
*Methods highlighted were discarded from the analysis due to the lack of information available in the open literature		

The main objective of this study is to compare models that are easy and quick to apply and available. For that reason, only empirical correlations were investigated. Table 2 summarizes all empirical correlations used in this work, highlighting the main variable used, the weaknesses and strengthens.

Table 2. List of Empirical Correlations used in the current study

Model	Main Variables	Main Assumptions and Drawbacks
TNT Equivalent	Mass of fuel (M_{fuel}) Fuel Heat of Combustion (ΔH_{fuel}) Explosion yield factor (α_c) Distance from explosion center (r)	**Positive Aspects** Easy to use **Drawback/challenges** It compares a vapor cloud explosion (initially as deflagration) to a detonation type of regime, as a result of TNT explosion. Does not calculate flame speed and neglects effects from confinement and congestion regions
TNO Multi-energy	Volume Blockage Ratio (VBR) Obstacle Diameter (D) Flammable Cloud Length ($\mathrm{L_p}$) Laminar Flame Speed (S_L) Cloud Confinement (2D or 3D)	**Positive aspects** Relatively easy to apply Maximum overpressure is based on the flame speed which is a function of the listed variables. Only confined and/or congested regions are included in the calculation **Drawback/challenges** It assumes uniform congested levels and there are no limiting values for Pmax.
PES	Obstacle Diameter (D) Distance between obstacle (x) Flammable Cloud Radius (R) Laminar Flame Speed (S_L) Laminar flame thickness (δ)	**Positive aspects** Maximum overpressure is based on the flame speed which is a function of the listed variables. There is a limiting value for Pmax **Drawback/challenges** It assumes uniform congested levels. It assumes central ignition (spherical shape explosions) It requires fitting models to estimate empirical factors a and b
CAM 2	Area blockage ratio (ABR) Distance between obstacles (x) Number of obstacle rows (N)	**Positive aspects** Relatively easy to use

	Laminar Flame Speed (S_L) Laminar flame thickness (δ)	Maximum overpressure is based on the flame speed which is a function of the listed variables. **Drawback/challenges** It assumes uniform congested levels. It does not estimate flame speed
BST	Laminar Flame Speed (S_L) Volume Blockage Ratio (VBR) Confinement (2D, 2.5D, and 3D)	**Positive Aspects** Easy to use Quick Takes into account some geometrical details Handle multi-ignition point **Drawbacks/challenges** Can be over conservative Does not account for the real cloud size
Melton and Marx	Laminar Flame Speed ((S_L) Volume Blockage Ratio (VBR)	**Positive Aspects** Easy to use Quick Takes into account some geometrical details Handle multi-ignition point **Drawbacks/challenges** Assume uniform congested levels
Li et al (2014) Correlation[18]	Area blockage ratio (ABR) Volume blockage ratio (VBR) Laminar Flame Speed (S_L) Average obstacle size (D)	**Positive aspects** Relatively easy to apply Maximum overpressure is based on the listed variables. Only confined and/or congested regions are included in the calculation **Drawback/challenges** It assumes uniform congested levels and there are no limiting values for Pmax.

3 Experimental data used as basis in this work

The experimental data used in this paper is from the tests conducted by a joint SRI/Gexcon [22, 23] which is summarized in Table *3* . Tests were performed using an experimental test facility with geometries similar to a full-scale petrochemical facility, where flame acceleration can occur.

Obstacles inside the facility were designed to represent typical congestion that can cause acceleration of the flame front through homogeneous mixtures of flammable gas (*i.e.*, methane or propane with air).The Modular Flame Acceleration Test facility was made up of a set of 30 congestion modules. The modular form gave flexibility in arranging the orientation of the obstacles to the facility geometry. This flexibility enhanced control in achieving the desired environment, including overpressure range, areal variation of the overpressure within the facility, and flame speed. Each module measured approximately 3.7 m by 3.7 m by 3.7 m. The modules were designed so that the congestion level could be adjusted by populating the module with pipes. Four different test configurations were used in this study: a) the 24-module "low congestion", b) the 30-module "low congestion", c) the 30-module "high congestion", and d) the 14-module "high congestion" configurations.

Table 3. Summary of all experimental conditions tested in the facility with propane and methane-air mixtures

No.	Fuel	**Equivalent Ratio**	**Congestion**	**Modules**	**Pmax (barg)**	**Maximum Flame Speed (m/s)**	**Combustion Regime**
5[a]	Propane	1.1	Low	24	39.4	1790	DDT
6[a]	Propane	1.1	Low	24	20.2	1760	DDT
7[b]	Propane	1.05	Low	24	44.5	1680	DDT
8[b]	Propane	1.05	Low	24	12.8	1680	DDT
9	Methane	0.95	Low	30	0.1	85	Slow Deflagration
10	Propane	0.8	Low	30	0.05	70	Slow Deflagration
11	Propane	1.35	Low	30	0.14	135	Fast Deflagration
12[a]	Propane	1.1	Low	24	21.0	1750	DDT
13	Methane	1.05	High	30	0.5	250	Fast Deflagration
14	Propane	0.9	High	30	21.6	1790	DDT
15	Propane	1.35	High	30	52.6	1720	DDT
16	Methane	1.05	High	30	15.6	830	Choked

17[c]	Methane	1.05	High	14	0.05	80	Slow Deflagration

Notes:

[a,b] Tests marked with letters presented similar experimental conditions

[c] Test 17 was excluded from the analysis because analysed the impact of suppression systems in the early stage of flame propagation.

Flame speed was determined via three different measurement techniques:

1. direct flame measurement using ion probes (partly unreliable)
2. direct flame tracking using the high-speed video
3. flame tracking using image gradient post processing.

4 Results and Discussion

This section is organized in three different estimated parameters: DDT predictability, source overpressure, and flame speed estimation. At the moment of this study, the data for overpressure at relative distance is not publicly available and, therefore, it is excluded from this analysis.

Table 4. List of parameters calculated by each model

Model	Calculated Parameters			
	Overpressure at relative distance	Flame Speed	Source Overpressure	DDT Potential
TNT Equivalent	X			
TNO MEM	X		X	X[a]
CAM 2	X		X	X[a]
BST	X	X	X	X
PES	X	X	X	X[b]
Melton and Marx Method	X	X	X	X
Li et al			X	X[a]

Notes:

a. Potential for DDT is assessed based on estimated overpressure. If overpressure exceeds 5 barg, then detonation is expected.
b. Potential for DDT is assessed based on estimated flame speed. If estimated flame speed exceeds the sonic velocity in the unburned mixture, then detonation is expected.

4.1 DDT Predictability

An initial analysis of the DDT predictability of each model was conducted using their original guidelines (see *Table 5*). Experiments with similar conditions are grouped in the same column. For methods that calculate source overpressure, DDT is assumed possible for case for which source pressure exceeds 5 barg. On the other hand, for methods that calculate flame speeds, DDT is considered probable when flame speed exceeds the sonic speed in the unreacted mixture.

It is interesting to observe that CAM 2 was the only method able to predict DDT for all cases that experienced this phenomenon. On the other hand, this model also highlights a potential for DDT in experiments with methane and high congestion (test 13,16, and 17). This is mainly due to the high dependency of the model on the obstruction parameters. It is important to have in mind that DDT for methane-air mixtures is extremely improbable, but this can be used as an indicator for flame acceleration.

The PES model only predicts DDT for tests with high congestion. Similar to CAM 2, PES has an exponential dependency with congestion parameters. The TNO MEM predicted DDT correctly for one test with propane-air mixture in high congestion.

Contrary to the other methods, BST and Melton and Marx model fail to predict DDT for all cases. This is because they exclude the possibility of DDT for fuels with medium reactivity such as propane [3].

Table 5. Results for DDT predictability based on original guidelines for each method. Cells marked by "x" indicates that DDT is possible. Green shade represents correct prediction and orange shade incorrect prediction.

	Tests with Propane						Tests with Methane			
	DDT				No DDT		No DDT			
	5,6,12	7,8	14*	15*	10	11	9	13*	16*	17*
TNO MEM	🟧	🟧	🟩 x	🟧	🟩	🟩	🟩	🟧 x	🟧 x	🟧 x
PES Model	🟧	🟧	🟩 x	🟩 x	🟩	🟩	🟩	🟧 x	🟧 x	🟧 x
CAM 2	🟩 x	🟩 x	🟩 x	🟩 x	🟩	🟧 x	🟩	🟧 x	🟧 x	🟧 x
BST 3	🟧	🟧	🟧	🟧	🟩	🟩	🟩	🟩	🟩	🟩
Melton and Marx	🟧	🟧	🟧	🟧	🟩	🟩	🟩	🟩	🟩	🟩
Li et al	🟧	🟧	🟩 x	🟧	🟩	🟩	🟩	🟩	🟩	🟩
* Tests with high VBR (high congestion)										

Modifications to the listed methods, except CAM 2, were suggested based on this analysis and the comparison with flame speed results (see section 4.2). Results originated from the final guidelines are presented in from the final guidelines are presented in Section 4.3.

4.2 Flame Speed Comparison (deflagrative part)

Flames speeds results from PES model, BST, and Melton and Marx method were compared experimental results. For tests in which DDT occurred, only the deflagrative part was considered.

PES Model

Figure 1 shows the predicted values obtained from PES model versus experimental data. A big discrepancy was observed between the results for high congestion values. In those cases, congestion parameters were used based on current guidelines: 0.3m for obstacle spacing (x) and 0.5 for obstacle size over obstacle spacing (y/x). This discrepancy was greatly reduced when both parameters were modified with the actual values of 0.6 m and 0.3 m, respectively.

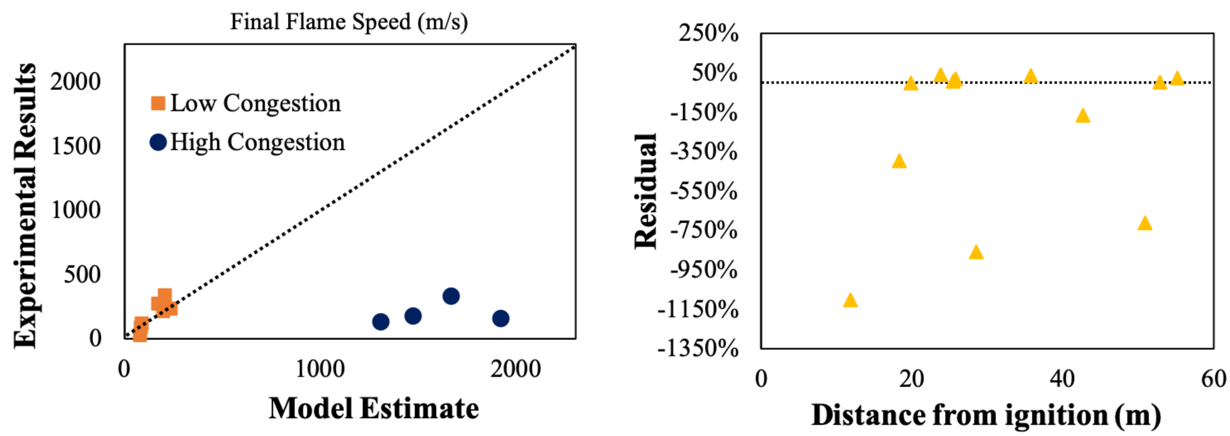

Figure 1. Comparison between predicted flame speed from PES model and experimental results, considering the deflagrative part (left -hand side), and the residual analysis (right-hand side). Congestion parameters are based on the method recommendations

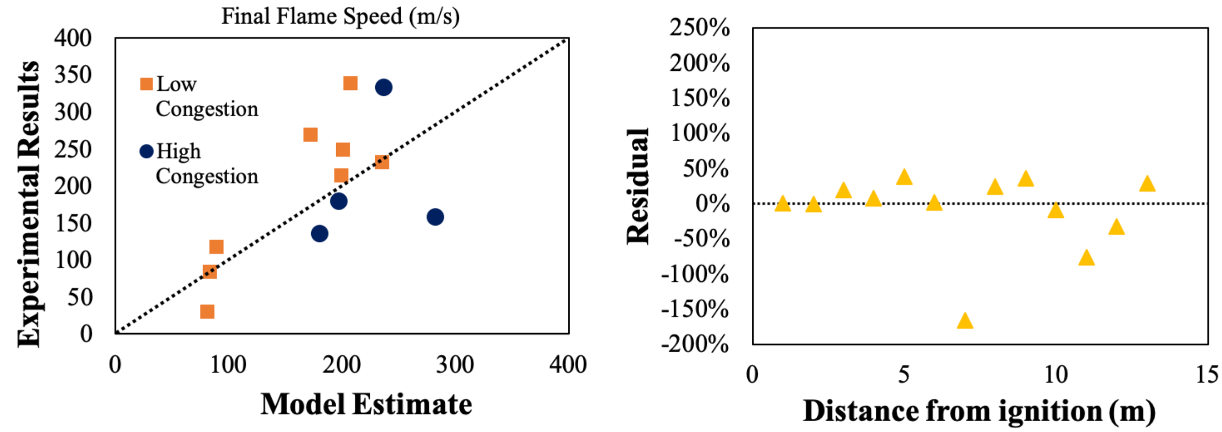

Figure 2. Comparison between predicted flame speed from PES model and experimental results, considering the deflagrative part (left -hand side), and the residual analysis (right-hand side). Congestion parameters were calculated using real parameters.

Melton and Marx Model

The Melton and Marx model combines the equation originated from MERGE experiments with the BST method to calculate flame speeds within a congested region. Although the results from this model were satisfactory using the normal guidelines (see Figure *3*), predictions were improved using a modified version (see Figure *4*). This modification simply consists of using the original values of Mach number (M_f) defined by Tang (ref needed). This new value are listed Table *6* and its applicability also improve the prediction of DDT as shown in section 4.3.

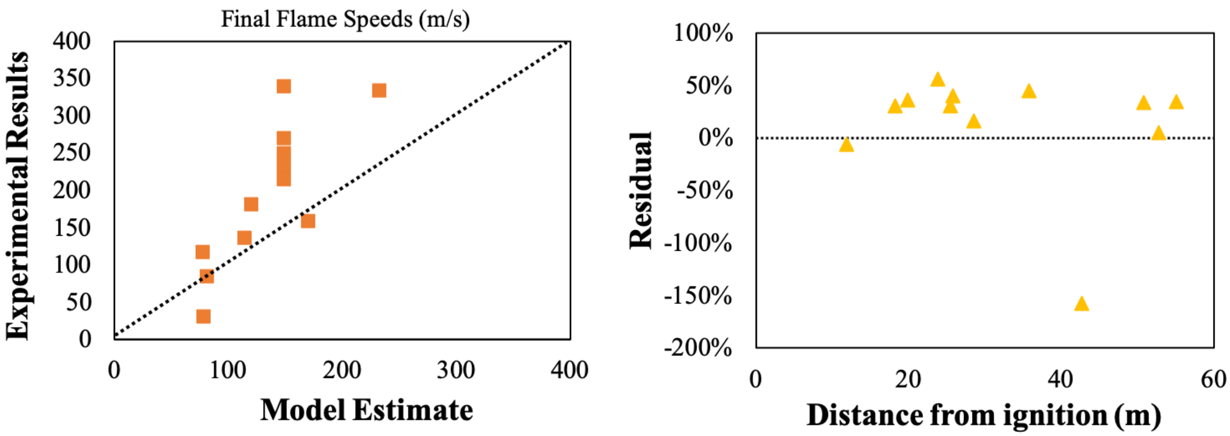

Figure 3. Comparison between predicted flame speed from Melton and Marx model and experimental results, considering the deflagrative part (left -hand side), and the residual analysis (right-hand side). Limiting Mach number (Mf) is calculated based on the method recommendations.

Table 6. Modified maximum Mach number (Mf) for flame speed calculation using Melton and Marx model

	Fuel Reactivity	Obstacle Density		
		H	M	L
2D Flame	H	5.3	5.3	0.81
	M	2	0.89	0.66
	L	0.89	0.66	0.13
2.5D Flame	H	5.3	5.3	0.66
	M	1.4	0.76	0.41
	L	0.7	0.49	0.09
3D Flame	H	5.3	5.3	0.5
	M	0.7	0.62	0.17
	L	0.48	0.32	0.06

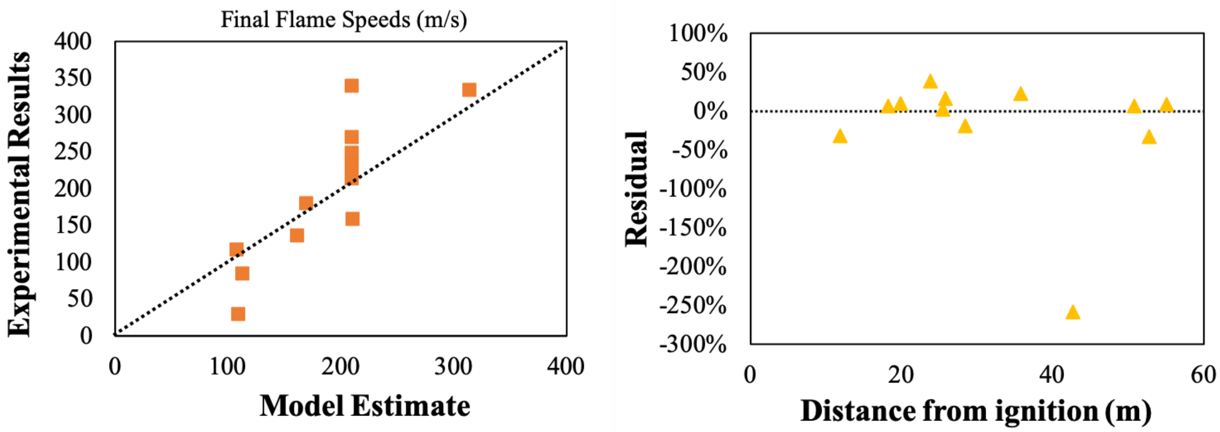

Figure 4. Comparison between predicted flame speed from Melton and Marx model and experimental results, considering the deflagrative part (left -hand side), and the residual analysis (right-hand side). Limiting Mach number (Mf) was modified based on the conversion between Mw and Mf published by Tang

4.3 DDT Predictability with Modified Guidelines

The prediction of DDT was improved for almost all the models used in this study, except for the one presented by Li et al because the number of data was scarce to proposed a significant change (see Table *7*).

Table 7. Results indicating the predictability of DDT using the modified version of each model guideline. Cells marked by "x" indicates that DDT is possible. Green shade represents correct prediction and orange shade incorrect prediction. Cells with* indicate suggested an improved result.

	Tests with Propane						**Tests with Methane**		
	DDT				No DDT		No DDT		
	5,6,12	7,8	14	15	10	11	9	13	16
TNO MEM	🟩 x*	🟩 x*	🟩 x	🟧	🟩	🟩	🟩	🟧 x	🟧 x
PES Model	🟩 x*	🟩 x*	🟩 x*	🟩 Def and DDT*	🟩	🟩	🟩	🟩 Def and DDT*	🟩 Def and DDT*
CAM 2	🟩 x	🟩 x	🟩 x	🟩 x	🟩	🟧 x	🟩	🟧 x	🟧 x
BST 3	🟩 Def and DDT*	🟩 Def and DDT*	🟩 Def and DDT*	🟩 Def and DDT*	🟩	🟩	🟩	🟩 Def and DDT*	🟩
Melton and Marx	🟩 Def and DDT*	🟩 Def and DDT*	🟩 Def and DDT*	🟩 Def and DDT*	🟩	🟩	🟩	🟩 Def and DDT*	🟩
Li et al	🟧	🟧	🟩 x	🟧	🟩	🟩	🟩	🟩	🟩

For TNO MEM, the current guide for overpressure prediction in elongated clouds consist first in estimating ΔP for the smallest side. If this value exceeds $30kPa$, then it is suggested to calculate for the longest flame path. The initial value of $30kPa$ was selected randomly, without experiment validation. For that reason, and based on the current data, the authors of this paper recommend reducing the threshold to 25kPa. This slight reduction enables a better prediction of DDT potential and flame acceleration.

For BST, PES and Melton and Marx, a new guide for DDT prediction was applied following the Mach number ranges proposed by Geng *et al.* [19]:

- $M_f < 0.6$, only deflagration is expected
- $0.6 \leq M_f < 0.9$, both deflagration and DDT are possible
- $M_f \geq 0.9$, DDT is expected

Using this new guidance improved considerably the prediction for all those three methods.

4.4 Source Overpressure (deflagrative part)

Lastly, Table 8 shows the comparison between the overpressure estimated from each model and the median value from the experimental results, deflagrative wave only. As expected, the TNT model originated the most conservative results. This model assumes that a percentage of the flammable cloud detonates. This is not very good given that detonation and deflagration as completely different phenomena. Both TNO MEM and CAM 2 originated over conservative results (more than 1,000%) for similar cases.

Table 8. Comparison (in percentage) between overpressure estimated from each model and experimental values (median value)

Methods	Tests with DDT (deflagrative section)							Tests without DDT				
	5	**6**	**7**	**8**	**12**	**14**	**15**	**9**	**10**	**11**	**13**	**16**
TNT	8E3%	1E4%	2E3%	1E4%	4E4%	9E3%	3E4%	2E5%	6E5%	2E5%	1E5%	5E5%
TNO MEM	239%	649%	978%	666%	3E3%	55%	2E3%	1E4%	5E4%	1E4%	2E4%	1E3%
BST	-42%	-10%	58%	12%	185%	-33%	25%	358%	1E4%	359%	496%	508%
PES Model	-21%	22%	111%	50%	285%	-15%	122%	835%	3E3%	990%	1E4%	327%
CAM 2	188%	357%	685%	458%	2E3%	318%	1E3%	4E4%	2E4%	7E3%	5E3%	2E3%
Melton and Marx	-42%	-10%	58%	12%	185%	-33%	25%	358%	1E3%	359%	496%	508%
Li et al	-77%	-36%	-16%	-40%	168%	-98%	47%	2E3%	9E3%	2E3%	2E3%	-65%

5 Conclusion

This paper reviews the most common and new methods available for DDT prediction and overpressure estimation in large unconfined vapor cloud. Initially, using their respective original guidance, only CAM 2 was able to accurately predict DDT for the cases analyzed. For that reason, the authors proposed slight modification when utilizing each model, improving their performance. It interesting to observe that simple methodologies, such those one reviewed, can be applied to predict DDT for large structures.

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