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Assessing Unconfined Vapor Cloud Explosions (UVCE) Physical Effects: A Software Built for Modelling with BST Methodology

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Anahtar Kelimeler

Yangın ve Patlama Analizi
Risk Değerlendirme
Tehlike Değerlendirme
Büyük Endüstriyel Kazalar

Graphical/Tabular Abstract (Grafik Özet)

The calculation of physical effects of unconfined vapor cloud explosions (UVCE), which are caused by explosive atmosphere, is important for risk assessment studies. In this study, an overpressure calculation software called ExCALc has been coded for use in UVCE risk assessment studies. ExCALc uses Baker-Strehlow-Tang (BST) model. / Patlayıcı atmosferin neden olduğu sınırlandırılmamış buhar bulutu patlamalarının (UVCE) fiziksel etkilerinin hesaplanması, risk değerlendirme çalışmaları için önemlidir. Bu çalışmada, UVCE risk değerlendirme çalışmalarında kullanılmak üzere ExCALc adı verilen bir fazla basınç hesaplama yazılımı kodlanmıştır. ExCALc, Baker-Strehlow-Tang (BST) modelini kullanır.

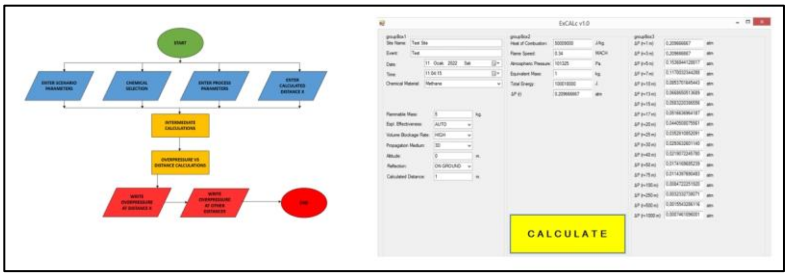

***Figure A**: ExCALc algorithm and screen image / **Şekil A:**. ExCALc algoritması ve ekran görüntüsü*

Highlights (Önemli noktalar)

- *UVCE etki modellemeleri yapılan bir yazılım geliştirilmiştir. / A software that models UVCE effects has been developed*
- *Yazılım; kütle, ortam geometrik özellikleri, kimyasal madde özellikleri ve rakıma göre atmosfer basıncı gibi etkenleri dikkate alarak hesaplama yapmaktadır. / The software makes calculations by considering factors like mass, geometrical properties of the medium, chemical properties and atmospheric pressure related to altitude.*
- *Yazılım; Patlamadan Korunma Dokümanı gibi projelerde kullanılabilecek şekilde Fazla Basınç sonuçlarını hesaplamaktadır. / The Software calculates overpressure results which can be used in projects like Explosion Protection Documents.*

***Aim (Amaç):** The aim of the study is to develop a software to evaluate explosion effects properly to be used in explosive atmosphere risk assessments. / Çalışmanın amacı, patlayıcı ortam risk değerlendirmelerinde kullanılabilecek, paylama etkilerini uygun bir şekilde değerlendiren bir yazılım geliştirmektir.*

***Originality (Özgünlük):** The capabilities of the output software of this study is very rarely encountered in free to use process safety solutions of its kind and has unique features like calculation atmospheric pressure related to altitude. / Bu çalışmanın çıktı yazılımının yetenekleri, kendi türünde ücretsiz proses güvenliği çözümlerinde çok nadiren karşılaşılır ve rakım ile ilgili atmosferik basıncın hesaplanması gibi yeni özelliklere sahiptir.*

***Results (Bulgular):** The final RMSE value of comparison samples (sample size of 392 calculations) was found to be 2.5637 × 10^{-3}. / Karşılaştırma örneklerinin nihai RMSE değeri (392 hesaplamalı örneklem büyüklüğü) 2,5637 × 10^{-3} olarak bulunmuştur.*

***Conclusion (Sonuç):** The prepared code is able to predict explosion overpressure for vapor clouds with a very small margin of error. / Hazırlanan kod, buhar bulutları için patlama fazla basıncını çok küçük bir hata payı ile tahmin edebilmektedir.*

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Abstract

The calculation of physical effects of unconfined vapor cloud explosions (UVCE), which are caused by explosive atmosphere, is important for risk assessment studies. During the evaluation of explosive atmospheres, effects of a possible explosion are determined in order to take safety measures. There are various algorithms for calculating the overpressure. In physical effect calculations, evaluation of the surrounding environment and chemical reaction are important criteria for accuracy of the results. Usually, a large portion of risk assessment studies neglect overpressure damage assessment as these algorithms cannot be understood or implemented easily due to difficulties in usage. There are various software used in calculating explosion overpressure, however these software generally are run without assessing operating limits and scenario parameters correctly. Thereby, explosion effects cannot be evaluated properly in many explosive atmosphere risk assessments. Taking this as the basis for our aim, an overpressure calculation software called ExCALc has been coded for use in UVCE risk assessment studies. ExCALc uses Baker-Strehlow-Tang (BST) model. The parameters are input in a user-friendly way and the scenario results are calculated for varying distances. It is thought that for complex methodology used in assessments, simplifying tools will benefit industrial safety in the long term.

Sınırlandırılmamış Buhar Bulutu Patlamalarının (UVCE) Fiziksel Etkilerinin Değerlendirilmesi: BST Metodolojisi ile Modelleme İçin Oluşturulmuş Bir Yazılım

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Öz

Patlayıcı atmosferin neden olduğu sınırlandırılmamış buhar bulutu patlamalarının (UVCE) fiziksel etkilerinin hesaplanması, risk değerlendirme çalışmaları için önemlidir. Patlayıcı ortamların değerlendirilmesi sırasında, güvenlik önlemlerinin alınması amacıyla olası bir patlamanın etkileri belirlenmektedir. Fazla basıncı hesaplamak için çeşitli algoritmalar vardır. Fiziksel etki hesaplamalarında, çevredeki ortamın ve kimyasal reaksiyonun değerlendirilmesi, sonuçların doğruluğu için önemli kriterlerdir. Genellikle, risk değerlendirme çalışmalarının büyük bir kısmı, kullanımdaki zorluklar nedeniyle bu algoritmalar kolayca anlaşılamadığı veya uygulanamadığı için aşırı basınç hasar değerlendirmesini ihmal eder. Patlama fazla basıncının hesaplanmasında kullanılan çeşitli yazılımlar vardır, ancak bu yazılımlar genellikle işletme limitleri ve senaryo parametreleri doğru bir şekilde değerlendirilmeden çalıştırılır. Bu nedenle, birçok patlayıcı atmosfer risk değerlendirmesinde patlama etkileri düzgün bir şekilde değerlendirilememektedir. Amacımızın temelinden yola çıkarak, UVCE risk değerlendirme çalışmalarında kullanılmak üzere ExCALc adı verilen bir aşırı basınç hesaplama yazılımı kodlanmıştır. ExCALc, Baker-Strehlow-Tang (BST) modelini kullanır. Parametreler kullanıcı dostu bir şekilde girilir ve senaryo sonuçları değişen mesafeler için hesaplanır. Değerlendirmelerde kullanılan karmaşık metodoloji için araçların basitleştirilmesinin uzun vadede endüstriyel güvenliğe fayda sağlayacağı düşünülmektedir.

1. INTRODUCTION (GİRİŞ)

Flammable gases and liquids are widely used in various fields, not only in industry but also in our daily life. Some of the common ones can be summed as: fuels, solvents, alcohols etc. In terms of chemical risk factors of flammable gases and liquid vapors, one of the most important risks besides fire and other health-environmental effects is Gas / Vapor Cloud Explosions that may occur as a result

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of ignition of the explosive atmosphere or cloudy dispersions where gas is homogeneously mixed with air as a flammable mixture in mainly gaseous form. This mixture is called Explosive Environment, and the explosion of these environments is called Vapor Cloud Explosion or Unconfined Vapor Cloud Explosion if it occurs in the open area [1].

Within the scope of Occupational Health and Safety, the evaluation of the hazard and risks that explosive environments may pose has gained importance in recent years. Explosive environments caused by flammable gases, liquid vapors and dust clouds pose great risks in both industry and our daily living environment. In many countries, legislation backed risk assessment studies for explosive atmosphere stipulates that the hazardous zones of explosive environments should be determined and safety measures to be taken should be determined for each of these areas [2]. One of the most important steps in evaluating the risks of explosive environments is to determine the physical effects of the explosion that may occur as a result of possible ignition and to take safety measures to protect employees from these effects. As overpressure of a shock or pressure wave is potentially the most damaging effect of an explosion for considerable distances; calculating overpressure for a possible accident scenario where an explosion may occur becomes very important for these risk assessments. Usually, these assessments are applied to GIS media to show hazardous zones around surrounding points of interest (an example is given in Figure 1).

The most reliable assessment for these kinds of studies would be a quantitative assessment where the damage and probability are tied to real values. Usually for explosions, overpressure is calculated by blast – energy formulas and damage are assessed by empirical probit equations or by comparing the results to observations from previous studies where explosion damages for overpressures are reported. As these calculations have an important amount of mathematical load, usually several software that apply these formulas to obtain overpressure – damage results are used in such studies [1-2].

2.MATERIALS AND METHODS (MATERYAL VE METOD)

In physical impact modelling studies, the change of selected physical effect according to the distance of an event is investigated using various algorithms and methods. Explosions have various effects such as a shock - pressure wave, intense light and sound propagation, formation of a possible flame or a fireball. The most important explosion physical impact investigated in Major Industrial Accidents and Explosion Protection Risk Assessment studies are shock - pressure wave and its spread. During an assessment study to model these effects, the aim is to determine the change of pressure generated by the explosion, with increasing distance from the event center. There are several algorithms for calculating the overpressure effects that can be effective at very long distances depending on the size of the explosion. Commonly used and generally accepted ones are TNT Equivalent model, Multi-Energy model (TNO) and Baker-Strehlow-Tang (BST) model [3]. Of these, the TNT Equivalent model is mainly explosions of reactive explosives, where the phenomena are usually single centered and propagate in a uniform way. For multi-centered Vapor Cloud Explosions, the event usually depends on various other environmental factors like confinement and propagation medium. There are two widely used methods developed especially for these types of explosions. These are the Multi-Energy and BST methods, both of which are used for flares of gas-vapor cloud spreading over a large volume.

TNT Equivalent Method

TNT Equivalency is a very commonly used method for solid explosives for military purposes and TNT explosions are among the most observed and experimented ones. The shock overpressure varying with distance and associated with the propagating energy, which in turn is associated with the amount of explosive mass is observed with many field experiments. Therefore, made with gathered data from these tests, the overpressure vs. normalized distance curve of TNT blasts is usually well defined as shown in Figure 2 [3].

The main factor determining the level of overpressure in explosions is the amount of energy released as a result of the chemical reaction. In TNT Equivalent method, the amount of energy of the unit mass of the chemical examined (the lower heat of combustion: Lower Thermal Value resulting from the combustion) will be proportioned with the energy that will occur as a result of the explosion of the same amount of TNT. The next step involves finding the total energy resulting from the reaction; factor in the reflection, blast propagation to find a normalized distance (r’) to compare with maximum overpressure (Pmax) curve. The model assumes single value for overpressure and a point symmetric blast propagation [4].

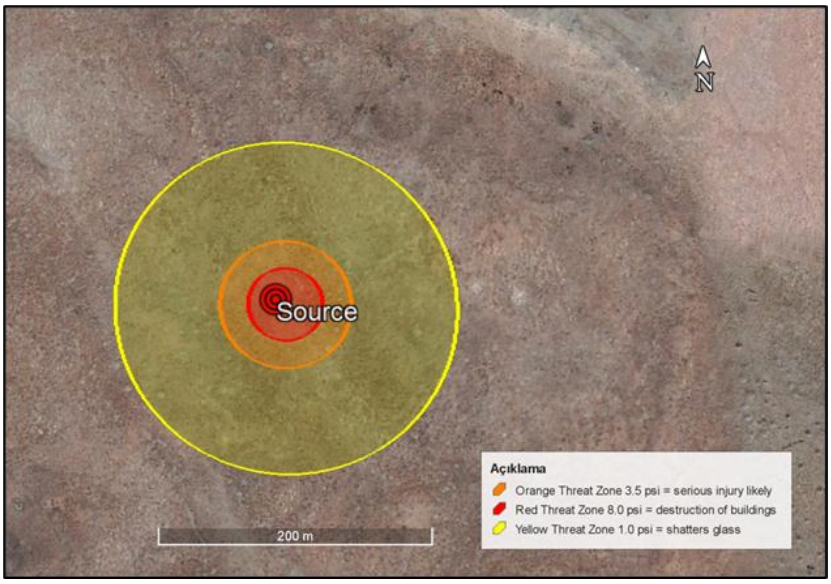

Figure 1. An exemplary explosion event overpressure - effects association (Örnek bir patlama olayı fazla basınç - etki ilişkisi)

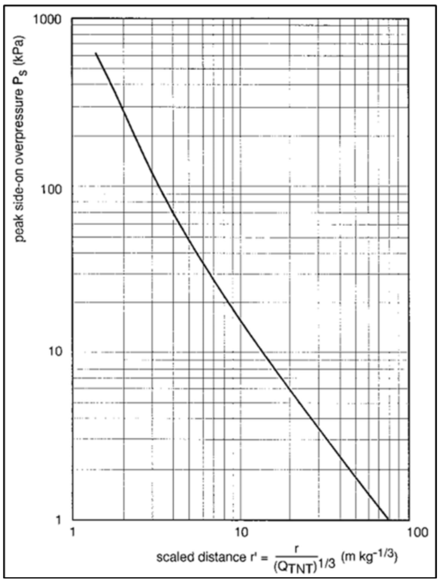

Figure 2. TNT Equivalent Model curve [3] (TNT Eşdeğer Modeli eğrisi)

Common factors for gas / vapor cloud explosions such as the presence of obstacles that may affect the overpressure, their location, the state of the ignition sources and the cloud's multi-centering are not considered in this method. For this reason, TNT Equivalent method is ideal for effect calculation in explosions of single center reactive explosives, but it is insufficient in gas / vapor cloud explosions.

TNO Multi Energy Method

In this method, developed by Van Den Berg (1985) at the TNO Institute, the methodology for determining the blast impact is basically based on the method of calculating the normalized distance derived from the amount of combustion heat. On the other hand, the main innovation of the method is 10 different distance - overpressure curves obtained by experiments that will correspond to 12 different scenarios that vary depending on the parameters: surface obstructions, parallel limiting structures and the ignition energy amount (Figure 3). These factors define the geometric parameters of a possible multi-centered and dispersed explosive atmosphere in an industrial facility. The assessment team would be interested in selecting the appropriate curve according to these scenario parameters to find the overpressure of the Vapor Cloud Explosion [5]. There has been a major improvement to Multi-Energy model by TNO as GAME model to determine the correct blast curve [6-7]. Characteristic overpressure – impulse curves using Multi-Energy method have been prepared by other researchers for ease of usage as both overpressure and impulse can be determined in one step making simulations of explosions simpler and faster [8].

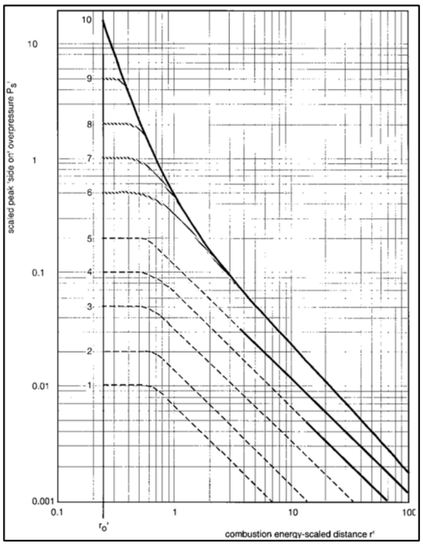

Figure 3. TNO Multi-Energy Model curves [5] (TNO Multi-Enerji Modeli Eğrileri)

Baker-Strehlow-Tang (BST) Method

The basic approach is the same as TNO Multi-Energy, however this time blast curves are determined directly by 9 blast shock wave (reaction front) velocities resulting from different environmental medium and chemical properties. Curve selection is made depending on the parameters of medium dimensions (2 dimensional, 3 dimensional etc.); presence of and blockage effect of obstacles and the reactivity of the chemical substance (classified by laminar burning rate) (Table 1). In this method curves are experimentally derived for each flame speed (Figure 4) [13].

The highest curve in this method is 5.2 MACH curve for DDT (Deflagration - Detonation Transition) which corresponds to curve number 10 in the Multi Energy method. Validation of calculated blast curves by comparing them with real experimental data from vapor cloud explosion studies have been made [9]. After the initial model was presented [10-11] the curves and methodology of BST was updated in later studies [12-13].

There have also been efforts to use the results of GAME methodology by TNO to associate with the blast curves of BST; a notable study has made the Quest Model for Estimation of Flames Speeds (QMEFS) which linked the GAME curve estimation P_{max} value to flame speed, therefore also enabling an approach to choose or extrapolate a realistic blast curve for BST model [14]. Also, the curves of BST were subjected for correction due to ground effect and validated in other studies [15].

Although events of Vapor Cloud Explosions are not expected to be as intense as full detonations; the factors such as confinement to smaller number of dimensions, increased blockage ratio or high combustive properties of the chemical will aid in speeding up the reaction, which may change a regular deflagration into a detonation [13]. Detailed calculation steps for this method are described in later section for software methodology.

Table 1. Flame Speeds (MACH) for different settings in Baker-Strehlow-Tang (Baker-Strehlow-Tang'da farklı ayarlar için Alev Hızları (MACH))

3D	**Congestion**		
Reactivity	***Low***	***Medium***	***High***
High	0.36	5.2	5.2
Medium	0.11	0.44	0.5
Low	0.026	0.23	0.34

2.5D	**Congestion**		
Reactivity	***Low***	***Medium***	***High***
High	0.47	5.2	5.2
Medium	0.29	0.55	1
Low	0.053	0.35	0.5

2D	**Congestion**		
Reactivity	***Low***	***Medium***	***High***
High	0.59	5.2	5.2
Medium	0.47	0.66	1.6
Low	0.079	0.47	0.66

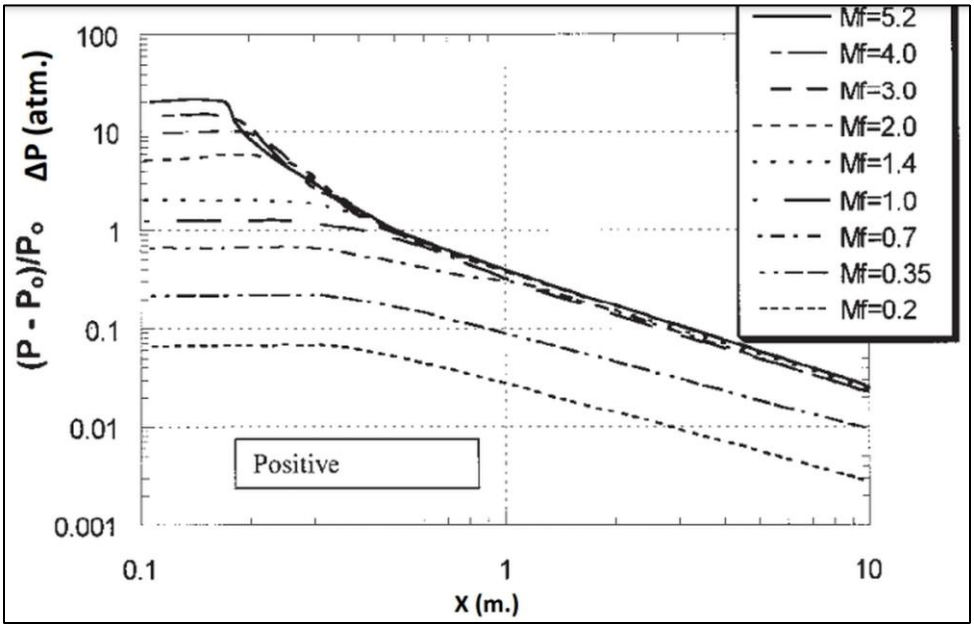

Figure 4. Curves for Baker-Strehlow-Tang (BST) [13] (Baker-Strehlow-Tang (BST) için eğriler)

3. COMPARISON OF MODELS (MODELLERİN KARŞILAŞTIRMASI)

There is a need to identify the result producing capacity of each model and compare them in order to determine the strong and weak points of the models. A previous study has compared these two models in terms of structural response and explosion damage and found that TNO Multi-Energy method predicts higher overpressures at shorter distances than BST and mostly agrees with BST results at longer distances [16-17].

There are two studies involving Hydrogen-Air mixture explosions that also use both methods for prediction and correlates them. The SRI H_2 explosion study performed a test in open space and the results were correlated with predictions of the methods. They found that inside near field both methods predicted 10-20% lower than and whole range values show good agreement with actual results. It is further argued that BST curves do not show a good prediction if the flame speed varies during propagation. Although this assumption can also be thought to be true for both methods as both of them have fixed curves for defined scenarios. The study found that Multi-Energy method results better fit the test data as the peak overpressure is well defined for the method than BST model [18].

Another study analyses the consequences of a scenario where VCE of H_2 that is leaked from a Hydrogen Holder in a chlor-alkali plant. The analyses were done with both Multi-Energy and BST methods and were correlated. The overpressure at 8 meters from the ignition centre, Multi-Energy method predicted 5.5 bars and BST method predicted 4.2 bars of overpressure. And at 25 meters from the ignition centre, overpressure values were found to be 0.4 bars for Multi-Energy and 0.3 bars for BST models whereas at 100 meters, overpressure values were 50 mbars for Multi-Energy and 90 mbars for BST models [19].

It can be generalized that Multi-Energy model predicts higher values in near field and at far field some analyses show good agreement while others show BST method predicting higher than Multi-Energy method. However experiences show the basic models of both TNO Multi-Energy (without using GAME method) and BST method are usually ambiguous in curve selection. Therefore if quantitative factors of maximum overpressure or flame speed cannot be determined for the scenario, choosing criteria like obstruction and propagation medium has to be determined well enough to choose the appropriate curve. And this results in varying results for different methods. Such an exemplary scenario with specific parameters was chosen for model comparison to analyse and evaluate the results (without using GAME method and/or BST maximum pressure – flame speed functional correlation).

Critical Loss of Containment (LOC) Event:

An atmospheric tank filled with Hexane has a feed line in which liquid Hexane is pumped for storage. A total failure of pump O-ring due to inadequate maintenance conditions is the expected scenario. This Loss of Containment (LOC) event will result with a Hexane spillage into the surrounding bund. This in turn will result in an evaporating pool and formation of a flammable vapor cloud that will spread and disperse due to atmospheric conditions. This cloud is thought to be indirectly ignited by an ignition source present in the surrounding environment sometime after the start of LOC event and will hence undergo a Vapor Cloud Explosion (VCE).

First, in order to determine the combustion mass of chemical, the cloud's dispersion has to be modelled. This was done with NOAA-EPA ALOHA software which uses typical spillage and evaporation models to calculate the mass/time parameter for the source of the cloud as described in its technical documentation [20].

Chemical Parameters:
Molecular Weight (MW): 86.18 g/mol
Density (liquid) (ρ_{liq}): 655 kg/m^3
Boiling Point (BP): 68.4 ^{o}C
Vapor Pressure: (@ 30 ^{o}C): ~0.25 bar
Lower Flammability Limit (LFL): %1.2 (v/v)
Upper Flammability Limit (UFL): %7.2 (v/v)
Process and Equipment Parameters:
LOC Equipment: O-ring failure of pump on the tank
Pressure in line (P): 8 bars
Temperature in line (T): 20 ^{o}C
Sectional area of the outflow (S): 5 mm^2 (derived from pump O-ring failure sectional area from IEC60079-10-1 standard [21].

Atmospheric conditions were chosen to represent a calm air midnight scenario with average humidity. Total outflow time at ignition moment (tLOC) is taken to be 30 minutes. ALOHA uses DEGADIS model[20] for dense cloud dispersions. As usual for all Vapor Cloud Explosion cases it defines the reference concentration as the Lower Flammability Limit (LFL) of the chemical, in order to find the maximum spread area possible. The model then determines a cloud average height and finds the total volume and mass of the cloud. The resulting dispersion from our scenario found the explosive mass as 3 kg. This value will be taken as the mass to ignite and undergo combustion to result into a vapor cloud explosion.

For the VCE set parameters and derived factors of the scenario are:

Chemical Parameters:
Chemical Material: N-Hexane (C_6H_{14})
Laminar Burning Speed (LBS): 50 cm/s
Reactivity: Medium
Heat of Combustion (lower) ($H_{c,low}$): 4.48 × 10^7 J/kg
Total vapor mass in combustion (M): 3 kg
Equivalent mass in explosive reaction (M_{eq}): 0.6 kg
Surrounding Environmental Parameters:
Ignition source is a general spark (no shock compression is present)
Altitude (Hgt): 0 meters
Atmospheric Pressure (P_0): 101325 Pa
Explosion on the ground
Reflection factor (ref): 2
Volume Blockage Ratio (VBR)
Obstructions: HIGH
Shock/Pressure Propagation Medium: 3D
Unconfined (no parallel plane confinement)

For BST model these settings point to:
Flame (Reaction Front) Speed: 0.5 MACH
And for Multi-Energy model this correlates to blast category 7 and 5th Blast Curve.
Total combustion Energy (E): 53702400 J
Real geometric distance: 10 meters
Normalized Distance (r' – X): 1.23568 meters
Overpressure (BST model) (ΔP): 148 mbar
Overpressure (Multi-Energy model) (ΔP): 101 mbar

The calculations done with set scenario parameters (and some chosen parameters of environmental propagation to correlate between two methods) found overpressure (ΔP) values of 148 mbar for BST method and 101 mbar for TNO Multi-Energy method. Not reported here as it is the expected result: TNT Equivalent model almost always results in higher overpressure values. Results of BST model 0.5 MACH curve is plotted as an overpressure – distance diagram and is shown in Figure 5.

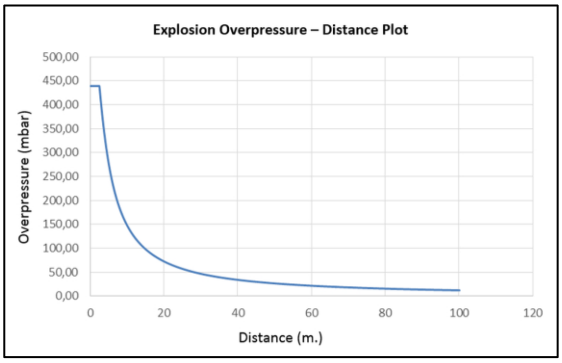

Figure 5. Overpressure – distance plot of the example scenario (Örnek senaryonun Fazla basınç – Mesafe grafiği)

Although both models use similar trending blast curves; when the correlating curves are analysed it can be seen that Multi-Energy model results are usually higher for the same normalized distance. This could have been also true for the curves used in the example scenario for which curve class 5 was selected (the highest available class from the class possibilities of a blast strength category 7 type scenario) to best identify the obstruction, confinement and ignition energy in Multi-Energy model and if the reactivity of the chemical was low then in BST model resulting curve would have been 0.35 MACH, which would produce lower overpressure results than the Multi-Energy model. However, as the chemical in the scenario has higher reactivity than a lower one like Methane gas, the resulting curve to be used is 0.5 MACH which produced higher overpressure results than the Multi-Energy model results. This is one of the most important factors to lean on BST model for Vapor Cloud Explosion overpressure modelling unless maximum overpressure and/or flame speed cannot be determined precisely. So it can be argued that although both models are derived from empirical data gathered from many experiments; BST defines the factors for scenario input understandably better (reactivity factor is present along with better definitions of the propagation environment, a better definition of Volume Blockage Ratio (VBR) etc.).

An important aspect of Vapor Cloud Explosions is the determination of the flammable mass. Several research have argued on different criteria for congested volume to be taken in calculations [3, 22]. Pitblado et al. (2014) have developed a detailed method for identifying the correct congestion volume which uses geometrical criteria that is defined with real site examples and this method, although developed for TNO Multi-Energy model, can also be used in conjunction with BST model.

There are also many research that defines the damage – impact to physical assets and/or health. These usually link the damage model (like Probit) to the overpressure values obtained from the consequence analyses and find the resulting damage ratio [23-25].

4. CODE FOR CALCULATING VCE OVERPRESSURE (VCE FAZLA BASINÇ HESAPLAMA KODU)

The need for a computerized executable code stems from the complexity and time consummation of all the previously mentioned calculations. Therefore, software specialized for methodological calculations are used regularly. Oftentimes some aspects of software, like scenario limitations, parameter selection criteria, output format are overlooked and all produced results are readily accepted as is. This raises questions of validity for various safety risk assessments involving complex methods.

For this study, a code was written to overcome this problem. Compiled into an executable named ExCALc software, the code was written in C# language for Windows desktop usage. It was prepared in Visual Studio environment. The software has built-in database for some common flammable chemicals and their parameters relevant to vapor cloud explosion physical effect calculations. The scenario definition includes an input to select the chemical (which in turn calls its properties from the database); inputs for environment geometry and the amount of material to go into combustion to result into an explosion. Basic algorithms for the execution steps are given in Figure 6.

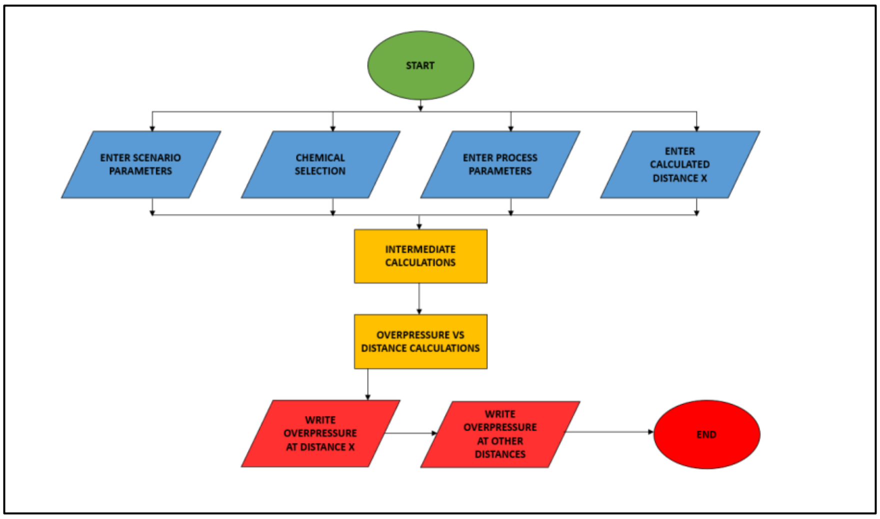

Figure 6. ExCALc basic algorithm and execution steps (ExCALc temel algoritması ve yürütme adımları)

For the methodology of calculation, the approach defined in BST is chosen as basis. This choice arises from facts gathered by comparing the VCE overpressure calculation methods described previously.

According to the method, first a reflection factor (ref) is chosen. For surface explosions as the ground will be mostly a rigid indestructible and unmoveable medium covering the lower half of the sphere of propagation, and hence the energy will only be able to do work on the upper half of the sphere, the ref factor will be a factor of ×2. If the explosion is taking place in air, then all directions will be free for work done and pressure propagation and therefore the ref factor will be ×1.

The next step includes the calculation of energy (Formula 1) that is formed by the combustion reaction that will result into the scenario explosion. This energy of combustion (E) is a factor of reflection factor (ref), lower heat of combustion ($H_{c,low}$) and equivalent mass of the flammable chemical taking part in the cloud (M_{eq}) which is usually a factor of 0.2 of total flammable mass in the cloud. This function is given in equation (1). The database includes values for lower heat of combustion ($H_{c,low}$) for some common flammables. Built-in database refers to DIPPR database for these values [26-28]. The database values for Hc,low are given in Table 2.

$$E = ref \times H_{c,low} \times M_{eq} \quad (1)$$

The next calculation step is finding the normalized distance (X) which is a function (Formula 2) of the real geometric distance (r), atmospheric pressure (P_0) and combustion energy (E).

$$X = r \times (P_0 / E)^{1/3} \quad (2)$$

Real distance (r) can either be user input or a differing parameter from 0 meters (the centre) to a maximum distance of outward reaches. It is also important to note the factor of atmospheric pressure (P_0) which will decrease with increasing altitude from the sea level. Many assessment studies overlook this factor to take it as some generic value like ~100000 Pascals to resemble sea level even though the scenario takes place far from the shore like an inland mountainous region. Therefore, on screen input for this factor is not the pressure value itself but the user is expected to enter the altitude from the sea level where the scenario will take place. Then the atmospheric pressure (P_0) is calculated from this altitude value. The last step includes selection of a typical blast curve (categorized with differing flame speeds) which according to experiments is dependent on these factors: the propagation medium (i.e. a 3D or 2D environment or in between), the ratio of blockage in the propagation volume (VBR) and the reactivity of the chemical itself (i.e. flammables like hydrogen and acetylene will be more reactive than slower reactives like methane). The reactivity is derived into 3 categories which the method chooses according to the laminar burning speed (LBS) values of the chemical. The database of chemicals included in the code has laminar burning speed (LBS) values for some common flammable materials to execute this categorization. The VBR is also categorized into 3 different settings. All these factors are typically found to result in explosive reactions with some typical flame speeds. The code will assess this flame speed and use the blast curve associated with that speed value. The curve will produce the overpressure ($\Delta P/P_0$) and is a function of normalized distance (X) [13].

Table 2. Database HC,low parameter values of chemicals (Veritabanı kimyasalların HC,düşük parametre değerleri)

Chemical	HC,low (J/kgK)	Chemical	HC,low (J/kgK)	Chemical	HC,low (J/kgK)
Methane	50009000	Isobutane	45613000	n-Butanol	33075000
Ethane	47794000	Cyclopentane	44636000	Dimethyl Ether	28703000
Propane	46357000	Etylene	47195000	Acetone	28548000
Butane	45752000	Propylene	45799000	Hydrogen	120971000
Pentane	45357000	Acetylene	48241000	Carbon monoxide	10112000
Hexane	44752000	Benzene	40170000	Ammonia	18646000
Heptane	44566000	Toluene	40589000	Gasoline	47000000
Octane	44427000	Xylene	4096100	Diesel Fuel	43400000
Nonane	44311000	Methanol	19930000	Natural Gas	54000000
Decane	44240000	Ethanol	28865000	Kerosene	43000000
Undecane	44194000	Isopropanol	30447000	Ethyl Acrylate	27630000
Dodecane	44147000	Formaldehyde	17259000	Ethyl Acetate	23510000
Cyclohexane	43450000	Acetaldehyde	24156000		

This product is the main output of the calculation code and the assessor can later use these output values to assess the expected damage by comparing it with some previous studies in which overpressure damage is well documented through experimental studies or real events. Short code blocks for the main calculation steps are given below:

```
Meq = M * Eff;
E = Ref * HC * Meq;
X = (r * (Math.Pow((Patm / E), (1.0 / 3.0))));
if (X < cX0) { dP = 1 * cD; };
if (X >= cX0) { dP = 1 * (cA * (Math.Pow(cB, (1.0
/ X))) * (Math.Pow(X, cC))); };
```

The output is given in two forms. The code uses the geometric distance (r) in two ways for these outputs. These are: 1) As there is a distance input for the user, this is used to calculate the exact overpressure at that point of distance from the event centre and 2) There are also a set of automatic calculations which take distance from 0 meters to a maximum of 1000 meters with increments of 0.1 meters to prepare a final distance – overpressure XY diagram. A calculation example is given in Figure 7.

5. VALIDATION OF CODE CALCULATIONS
(KOD HESAPLAMALARI DOĞRULAMALARI)

In order to validate the product results of the code, comparison approach with literature and an approach to compare code results with results from a different software that uses the same methodology (BST model) that can define a scenario with similar details are taken. There are many software that uses BST method for the calculation of side-on overpressure. Some examples include DNV PHAST, TNO EFFECTS, NOAA-EPA ALOHA. Almost all of them can calculate results for each step of a scenario starting from source LOC up to the various branches of the event tree like outflow, evaporation, dispersion, fire heat radiation, explosion overpressure, toxic concentration of cloud etc. Other than the usual consequence analysis of physical effects, damage definitions like death ratio, health effect ratios can also be calculated. It is not the aim of this study to compare these software as the aim is to develop a new code and validate it by comparison. As any of the above solutions are widely used and accepted in industry, the best and easily available one amongst them which is NOAA-EPA ALOHA is chosen for its ease of access.

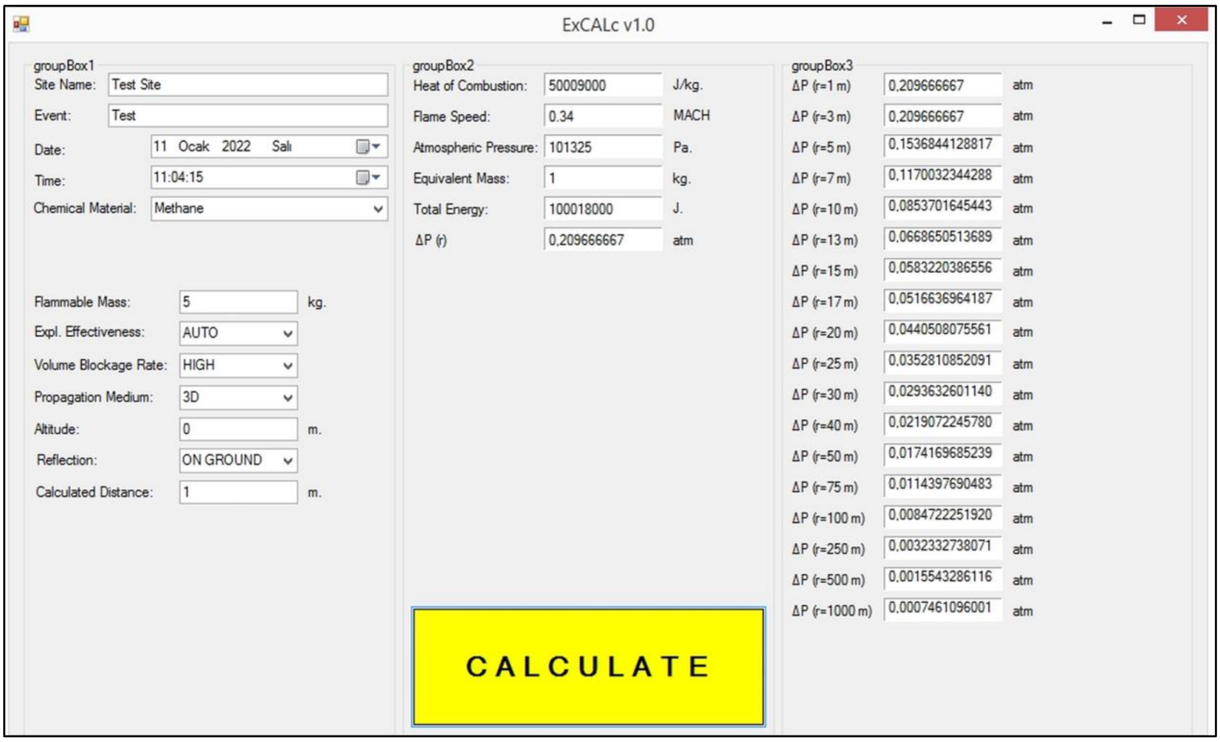

Figure 7. ExCALc screen image of a calculation example (Bir hesaplama örneğinin ExCALc ekran görüntüsü)

Literature comparison is made with two previous studies. Soman (2012) reports Hydrogen VCE overpressure values of 0.7, 0.3 and 0.09 atm. for 0.64, 1.06 and 4.25 meters of scaled distances respectively for 1.77 MACH curve [19]. As 1.77 MACH curve is not calculated in the code, the nearest one (1.6 MACH) is taken for comparison which produced results: 0.51, 0.29 and 0.057 atm. for the same set of scaled distances respectively. These results show good agreement with the general trend of overpressure change but as the curves are different, there are differences in near and far field results. Also, Kang (2010) reports Hydrogen VCE test results which are: 0.15, 0.065 and 0.028 atm. for 2, 4 and 7.5 meters of scaled distances respectively for the 5.2 MACH blast curve [18]. Using the same speed in ExCALc code the calculated results for comparison are: 0.155, 0.064 and 0.03 atm. for the same scaled distances respectively. These results show good agreement with the test values reported by Kang (2010).

For the tests 30 different scenarios, involving 3 different chemical materials are devised. Selected chemicals are Methane, Hexane and Hydrogen. These are selected to represent each class of reactivity for BST calculations. The scenarios for each chemical are 5 different explosive masses (0.01 kg., 0.1 kg., 1 kg., 10 kg. and 50 kg. for Methane; N-Hexane and 40 kg. for Hydrogen) for both congested and uncongested 3D environments. Each of them is run for 18 different distance values which are 1, 3, 5, 7, 10, 13, 15, 17, 20, 25, 30, 40, 50, 75, 100, 250, 500 and 1000 meters. A total of 540 calculations with unique scenario settings are run at first in ALOHA and then ExCALc and their results are compared. Out of the 540 calculations, only 392 of them produced meaningful results as rest of them were reported by ALOHA as insignificant. These scenarios are associated with lower mass and farther distances. Residual results of ALOHA and ExCALc runs are given in Table 3. Items marked in red indicate to values above 5 ‰.

For comparison, Root Mean Square Error (RMSE) is measured with residuals of observed ALOHA values and ExCALc estimated values for each unique scenario set. RMSE is described in Formula (3) where Yt is the observed value; Ȳt is the estimated value and T is the total sample size [29-30]. The sample size for comparison consists of outputs from the 392 scenarios that produced meaningful results.

$$RMSE = \sqrt{\frac{\sum_{t=1}^{T}(\bar{Y}_t - Y_t)^2}{T}} \qquad (3)$$

The final RMSE value was found to be 2.5637×10^{-3}. Majority of the differences are found in low obstruction medium Hydrogen scenarios at near the source fields. Although mean deviations are found to be low in general, the maximum deviation seen in scenarios is determined as 1.3397 %. This value is only detected in near field results of Hydrogen explosion scenarios in a low obstructed 3D propagation environment. There are several possible reasons for this deviation. There may be minor differences in the chemical database heat of combustion values, which ALOHA uses DIPPR licenced values. However, the main reason for the deviation is thought to be differences in curve fit function constants. Although for both applications, the constants are derived from the same source [13] and since the source does not include curves for every possible flame speed MACH number, the curves in-between the known ones are extrapolated. This extrapolation difference is notably detected in only a single flame speed of 0.36 MACH, which is associated with explosions of highly reactive chemicals (i.e. Hydrogen, Acetylene) in a low obstructed 3D environment. And for this curve, only the near source field values are affected and other values for farther distances are in an acceptable range. The other scenarios also use extrapolated curves and constants and results for these flame speeds are also in acceptable ranges both for near and farther from the source fields. It should also be noted that ALOHA only models high and low 3D propagation environments, which coupled with three classes of reactivity amounts to only 6 different possible flame speeds for scenarios. Except the 5.2 MACH DDT curve, all of them are extrapolated for in-between flame speeds which are not defined as a curve in the source literature.

Overpressure values are usually associated with expected damage using methods like probit curves in explosion risk assessment studies. Therefore, significant changes for damage ratio would be meaningful in these assessments. Even the maximum deviation observed in independent scenarios is unlikely to produce a meaningful change in expected damage ratios as the margin is too small and both solutions would predict similar damages. It can be deduced from these facts that the prepared code for this study is performing adequately to fulfil its mission.

Table 3. Residual results of ALOHA and ExCALc scenario runs (red cells indicate values above 5 ‰) (ALOHA ve ExCALc senaryo çalıştırmalarının artık sonuçları (kırmızı hücreler 5 ‰'nin üzerindeki değerleri gösterir))

		Distance (meters)																	
		1	**3**	**5**	**7**	**10**	**13**	**15**	**17**	**20**	**25**	**30**	**40**	**50**	**75**	**100**	**250**	**500**	**1000**
		3D / Low VBR / Methane																	
Mass (kg)	**0.01**	0.00051	0.00085	0.00144	0.00011														
	0.1	0.00020	0.00075	0.00206	0.00222	0.00426	0.00036	0.00024	0.00006	0.00091									
	1	0.00024	0.00038	0.00034	0.00039	0.00053	0.00044	0.00156	0.00307	0.00372	0.00063	0.00007	0.00017						
	10	0.00024	0.00024	0.00101	0.00006	0.00051	0.00020	0.00017	0.00014	0.00014	0.00013	0.00085	0.00092	0.00144	0.00041				
	50	0.00024	0.00024	0.00024	0.00024	0.00055	0.00085	0.00103	0.00078	0.00077	0.00096	0.00182	0.00155	0.00105	0.00201	0.00015			
		3D / High VBR / Methane																	
Mass (kg)	**0.01**	0.00183	0.00072	0.00134	0.00196	0.00307	0.00411	0.00271	0.00052	0.00035	0.00037	0.00044							
	0.1	0.00020	0.00370	0.00004	0.00081	0.00059	0.00158	0.00073	0.00117	0.00148	0.00225	0.00113	0.00012	0.00057					
	1	0.00366	0.00198	0.00355	0.00205	0.00010	0.00002	0.00063	0.00115	0.00054	0.00088	0.00109	0.00016	0.00235	0.00034	0.00003			
	10	0.00366	0.00366	0.00110	0.00001	0.00183	0.00072	0.00229	0.00055	0.00061	0.00067	0.00072	0.00112	0.00134	0.00129	0.00307	0.00037		
	50	0.00366	0.00366	0.00366	0.00122	0.00044	0.00200	0.00153	0.00047	0.00167	0.00319	0.00050	0.00078	0.00092	0.00008	0.00125	0.00425	0.00011	
		3D / Low VBR / N-Hexane																	
Mass (kg)	**0.01**	0.00171	0.00236																
	0.1	0.00101	0.00084	0.00051	0.00201	0.00232													
	1	0.00024	0.00063	0.00203	0.00023	0.00079	0.00038	0.00112	0.00153	0.00104									
	10	0.00024	0.00024	0.00078	0.00173	0.00171	0.00214	0.00096	0.00028	0.00212	0.00092	0.00236	0.00169						
	50	0.00024	0.00024	0.00024	0.00024	0.00014	0.00025	0.00070	0.00050	0.00127	0.00040	0.00071	0.00170	0.00067	0.00216				
		3D / High VBR / N-Hexane																	
Mass (kg)	**0.01**	0.00008	0.00000	0.00072	0.00023	0.00004	0.00205	0.00256	0.00126	0.00491									
	0.1	0.00000	0.00279	0.00271	0.00086	0.00168	0.00105	0.00141	0.00032	0.00222	0.00009	0.00029	0.00284	0.00426					
	1	0.00002	0.00201	0.00162	0.00046	0.00225	0.00039	0.00128	0.00174	0.00088	0.00160	0.00113	0.00088	0.00151	0.00445	0.00034			
	10	0.00002	0.00002	0.00175	0.00015	0.00008	0.00047	0.00359	0.00111	0.00321	0.00522	0.00000	0.00219	0.00237	0.00229	0.00004			
	50	0.00002	0.00002	0.00002	0.00072	0.00024	0.00101	0.00152	0.00101	0.00003	0.00144	0.00174	0.00367	0.00086	0.00036	0.00042	0.00137		
		3D / Low VBR / Hydrogen																	
Mass (kg)	**0.01**	0.00102	0.00010	0.00049	0.00058	0.00152	0.00072	0.00192	0.00235	0.00310	0.00043	0.00022	0.00035						
	0.1	0.01340	0.00271	0.00392	0.00056	0.00097	0.00018	0.00078	0.00152	0.00028	0.00075	0.00265	0.00088	0.00052	0.00062				
	1	0.01340	0.00096	0.00169	0.00009	0.00222	0.00054	0.00058	0.00011	0.00069	0.00086	0.00118	0.00099	0.00115	0.00080	0.00122			
	10	0.01340	0.01340	0.01340	0.00044	0.00102	0.00090	0.00165	0.00034	0.00502	0.00111	0.00132	0.00050	0.00155	0.00006	0.00152			
	40	0.01340	0.01340	0.01340	0.01340	0.00125	0.00148	0.00045	0.00161	0.00148	0.00015	0.00056	0.00056	0.00022	0.00026	0.00126	0.00096		
		3D / High VBR / Hydrogen																	
Mass (kg)	**0.01**	0.00051	0.00029	0.00089	0.00030	0.00246	0.00018	0.00032	0.00084	0.00053	0.00120	0.00077	0.00192	0.00082	0.00044	0.00024			
	0.1	0.00129	0.00131	0.00071	0.00084	0.00004	0.00103	0.00162	0.00088	0.00248	0.00017	0.00031	0.00074	0.00107	0.00126	0.00109	0.00017		
	1	0.00028	0.00111	0.00125	0.00158	0.00055	0.00030	0.00075	0.00027	0.00084	0.00161	0.00168	0.00134	0.00206	0.00082	0.00032	0.00204	0.00009	
	10	0.00028	0.00028	0.00537	0.00314	0.00310	0.00142	0.00029	0.00356	0.00118	0.00124	0.00205	0.00152	0.00089	0.00023	0.00246	0.00120	0.00082	0.00116
	40	0.00028	0.00028	0.00028	0.00028	0.00460	0.00121	0.00122	0.00171	0.00138	0.00282	0.00478	0.00007	0.00137	0.00097	0.00002	0.00020	0.00108	0.00018

6. CONCLUSIONS (SONUÇLAR)

Overpressure estimation is an important assessment where an explosion event is expected. This event can be as limited as an occupational safety issue (which may still pose a danger to life and/or health) to as large a one that can cause a major disaster. As an explosion is a violent and highly destructive event, capability to estimate based on live experimental observations beforehand is very limited for many sites and parties. Mathematical estimation based on empirical data or computational fluid dynamics have been and are still widely used tools for these assessments.

The prepared code associated with a user interface as a small software package is found to be useful for risk assessment arising from explosions as it is able to predict explosion overpressure for vapor clouds with a very small margin of error compared to industry regularly used software that is also used for this purpose amongst other assessment possibilities.

Whichever tool is used it should always be ensured that the physical variables and criteria for the explosion like mass or propagation environment must be chosen accurately by the professional making the assessment to obtain as realistic results as possible.

FUTURE WORK (GELECEK ÇALIŞMALAR)

Future works are planned for coding to involve calculation using several available research methods defined for overpressure – flame speed association; determination of correct VBR and congestion volume (therefore calculating the realistic mass).

AVAILABILITY OF DATA AND ASSETS (VERİ VE VARLIKLARIN KULLANILABİLİRLİĞİ)

The raw data for scenario runs and the software in Windows executable format are freely available upon correspondence.

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DECLARATION OF ETHICAL STANDARDS (ETİK STANDARTLARIN BEYANI)

The author of this article declares that the materials and methods they use in their work do not require ethical committee approval and/or legal-specific permission.

Bu makalenin yazarı çalışmalarında kullandıkları materyal ve yöntemlerin etik kurul izni ve/veya yasal-özel bir izin gerektirmediğini beyan ederler.

AUTHORS' CONTRIBUTIONS (YAZARLARIN KATKILARI)

***Tahsin Aykan KEPEKLİ*:** Devised the algorithm, researched the methods and coded them into a software. Also, conducted the test studies and analyzed the results.

Algoritmayı geliştirmiş, metotları araştırmış ve onları kodlayarak yazılım haline getirmiştir. Ayrıca, test çalışmalarını yapmış ve sonuçları analiz etmiştir.

CONFLICT OF INTEREST (ÇIKAR ÇATIŞMASI)

There is no conflict of interest in this study.

Bu çalışmada herhangi bir çıkar çatışması yoktur.

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