Potential for Hydrogen DDT with Ambient Vaporizers

J. Kelly Thomas†, Jihui Geng, and Oscar Rodriquez
Baker Engineering and Risk Consultants, Inc. (BakerRisk®)
3330 Oakwell Court, Suite 100, San Antonio, TX 78218-3024

Simon Jallais and Elena Vyazmina
Air Liquide R&D
1 Chemin de la Porte des Loges - Les Loges-en-Josas, 78354 JOUY-EN JOSAS

Derek Miller
Air Products
7201 Hamilton Boulevard, Allentown, PA 18195-1501

Bill Lindberg and Richard Pawulski
Air Liquide Large Industries U.S.
9811 Katy Freeway, Suite 100, Houston TX 77024

†Presenter E-mail: KThomas@BakerRisk.com

Abstract

The ignition of a hydrogen-air mixture that has engulfed a typical set of ambient vaporizers (i.e., an array of finned tubes) may result in a deflagration-to-detonation transition (DDT). Simplified curve-based vapor cloud explosion (VCE) blast load prediction methods, such as the Baker-Strehlow-Tang (BST) method, would predict a DDT given that typical ambient vaporizers would be rated as medium or high congestion and hydrogen is a high reactivity fuel (i.e., high laminar burning velocity).

Computational fluid dynamic (CFD) analysis of a single vaporizer of typical construction was carried out using the FLACS code to evaluate the potential for a DDT with a vaporizer engulfed by a hydrogen-air mixture at the worst-case concentration. This analysis showed that while significant flame acceleration occurs within the vaporizer, as expected, a DDT is not predicted. However, the analysis did indicate that a DDT may occur for two or more closely spaced vaporizers. This is relevant since multiple vaporizers are frequently present at industrial installations and are typically placed closely together to limit the required area. Spacing adjacent vaporizers further apart could preclude a DDT. However, specification of the spacing to preclude a DDT would require refined CFD analysis and/or testing, neither of which has been performed at this time.

This paper also discusses the application of simplified VCE blast load methods to ambient vaporizers engulfed in a flammable hydrogen-air cloud in order to illustrate the impact of a DDT.

Introduction

Vaporizers are employed on industrial sites to convert cryogenic liquids (e.g., hydrogen, nitrogen, etc.) into vapor for use in a process. The vaporizers of interest are finned tubes. Typically, a vaporizer consists of a number of vertically oriented finned tubes placed in close proximity in order to limit the vaporizer footprint. The vaporizer dimensions and the number and size of the finned tubes employed in a vaporizer depends on its service (i.e., gas vaporized, required flow rate, etc.) Multiple vaporizers are frequently utilized, with individual vaporizers typically separated by no more than several feet in order to limit the footprint of the vaporizer set.

An accidental hydrogen release could potentially interact with or engulf a vaporizer or set of vaporizers; a release could occur either from the liquid hydrogen supply or from downstream pressurized gas. The vaporizer structure (i.e., array of finned tubes) represents a congested volume, which could trigger a vapor cloud explosion (VCE) if filled with a flammable gas and subsequently ignited. If a hydrogen release near a congested volume is credible for a given operation, then a hydrogen VCE should be considered as a credible event when performing explosion consequence and risk assessments [1]. An approach to predict the resulting VCE blast loads is therefore needed in order to carry out such assessments at industrial sites employing vaporizers.

A typical vaporizer represents significant congestion level in terms of area blockage ratio (ABR), volume blockage ratio (VBR) or surface area to volume ratio (SA/V) due to the arrangement of finned tubes. The congestion level for a typical vaporizer would be classified as either medium or high under the Baker-Strehlow-Tang (BST) VCE blast load prediction method [2]. The BST method predicts a deflagration-to-detonation transition (DDT) at medium or high congestion levels for a high reactivity fuel (e.g., hydrogen) [3], and hence a vaporizer hydrogen-air VCE would be treated as a detonation. The prediction of a DDT for a medium congestion level with a high reactivity fuel under the BST method is based on testing performed by BakerRisk with ethylene and lean hydrogen mixtures [4, 5, 6]. The test rig used in these tests had dimensions of 48 feet (14.6 m) by 12 feet (3.7 m) by 6 feet (1.8 m) tall rig. The congestion employed in these tests was formed by a uniform array of 2-inch (5 cm) vertical pipes (pitch-to-diameter ratio of 4.1, area and volume blockage ratios of 23% and 4.2%, respectively); this would be classified as medium with the context of the BST method. Hydrogen-air mixtures were ignited at the rig center near grade level. Deflagrations resulted for hydrogen concentrations of 18% or less, a very fast deflagration was achieved at a concentration of 20%, and a DDT occurred with a concentration of 22%. Others have observed similar behaviour in hydrogen VCE tests. For example, Shirvill and Roberts [7] tested hydrogen in a congested 3 m by 3 m by 2 m high rig with congestion formed by 1-inch (2.54 cm) diameter pipes. A vertical array was placed in the bottom half of the rig, and a horizontal array in the top half. The mixture was ignited by a spark near the rig center. A near-stoichiometric H_2-air mixture underwent DDT near the edge of the rig.

If the flammable hydrogen-air mixture was restricted to the congested volume associated with a vaporizer or vaporizer set, the assumption of whether the VCE progressed as a high-speed deflagration or a detonation would have little impact on the VCE blast loads at moderate distances from the vaporizer (i.e., at most building locations). However, a detonation wave, once triggered by a DDT, can propagate through the remaining (i.e., unburned) flammable cloud [8, 9]. It is recognized that the detonation wave may fail before the edge of a flammable hydrogen-air cloud (i.e., at a higher concentration than the lower flammability limit), if the flammable cloud is too thin, or the concentration gradients are too large. A DDT that triggers a sustained detonation can therefore dramatically increase the VCE explosion energy for a hydrogen-air cloud which is much larger than a vaporizer, which would be the case for most postulated design-basis hydrogen release scenarios.

The lateral dimensions of a typical vaporizer (i.e., several meters) are less than rig length employed in the BakerRisk hydrogen DDT tests (i.e., 15 m). Hence, although the congestion level associated with a typical vaporizer is more severe than that of this test rig, it is possible that a DDT may not occur due to the decreased congested volume dimensions. Of course, the use of multiple closely spaced vaporizers increases the effective dimensions of the congested volume. A DDT evaluation for a typical vaporizer and vaporizer set was therefore carried out using the FLACS computational fluid dynamics (CFD) code. In order to illustrate the impact of whether or not a DDT occurs, a VCE blast load assessment was performed using the BST method for a hydrogen-air cloud resulting from a moderate liquid hydrogen release.

Effect on DDT on Predicted Blast Load

A ½-inch release of liquid hydrogen at a pressure and temperature of 150 psig and -410°F, respectively, was considered for the purposes of illustration. The postulated release was assessed using SafeSite$_{3G}$©, BakerRisk's consequence assessment and facility siting code. A Pasquill stability class B and a wind speed of 2 m/s was assumed for the dispersion. Figure 1 shows the upper flammability limit (UFL), lower flammability limit (LFL) and LFL/2 contours on a vertical cut plane through the center of the resulting hydrogen-air cloud. The corresponding flammable cloud volume is 130,000 ft^3. It should be clearly noted that larger releases and more severe weather conditions giving larger flammable cloud volumes are likely credible and would typically be considered in a risk analysis; that is, this flammable cloud volume should be viewed as moderate within the context of this illustration.

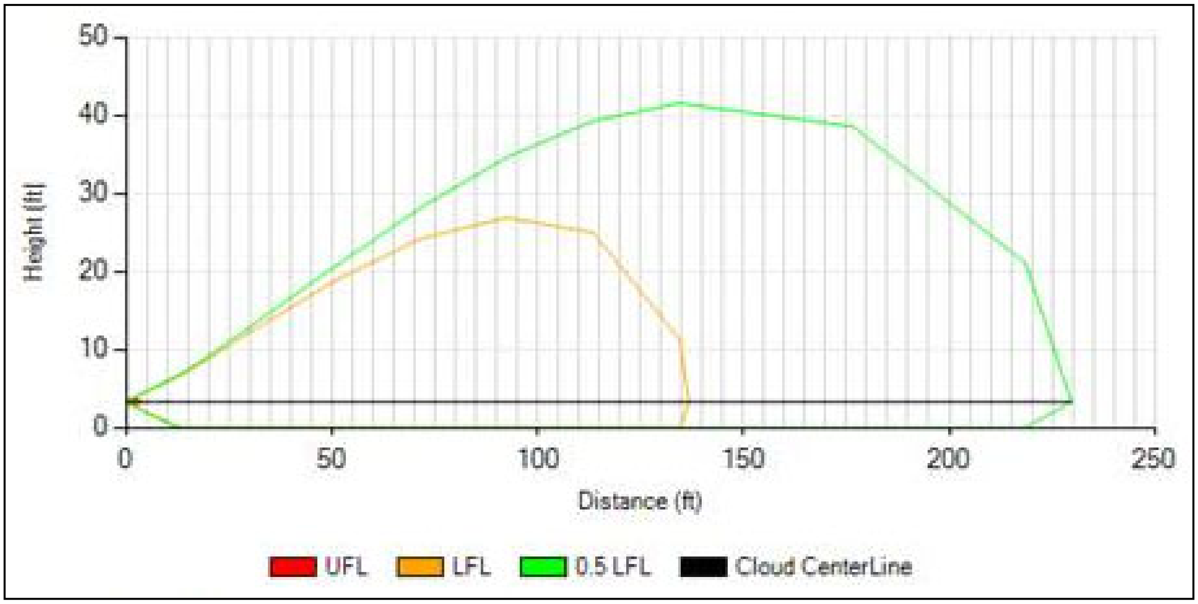

Figure 1. Flammable Hydrogen-Air Cloud for Example Release Scenario

For the purposes of the illustrative blast load evaluation, consider the flammable cloud and vaporizer arrangement shown in Figure 2. The flammable cloud is much larger than the vaporizer and engulfs it, with the vaporizer being the only congested volume within the flammable cloud. The ignition location is near the center of the flammable cloud and well outside the vaporizer. A low flame velocity flash fire (i.e., combustion without the generation of significant overpressure) would propagate out from the ignition location until the flame reached the vaporizer, at which point the flame would accelerate within the vaporizer due to the congestion presented by the finned tube array. If a DDT did not occur, then the flame would decelerate rapidly as it left the vaporizer (i.e., due to the absence of congestion outside the vaporizer), and the remainder of the flammable cloud would be consumed as a flash fire. However, if a DDT occurred within the vaporizer, then the resulting detonation wave would propagate outward from the vaporizer and consume the remaining flammable cloud (i.e., through the portion of the cloud capable of supporting a detonation, down to the leanest hydrogen concentration that supports detonation propagation).

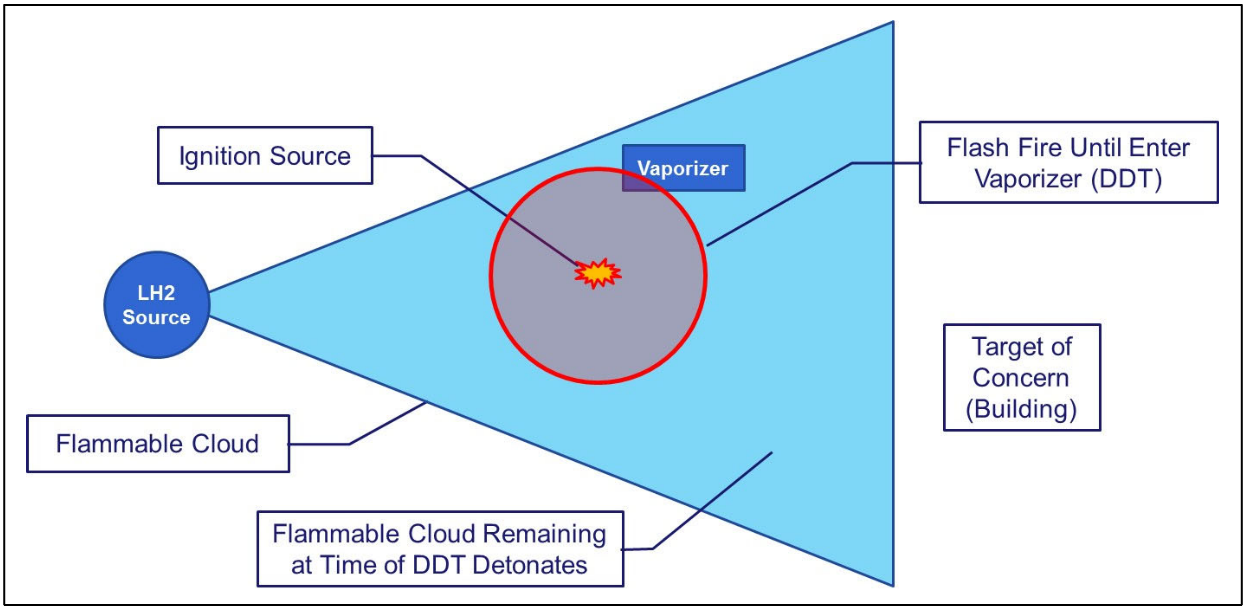

Figure 2. Illustrative Flammable Hydrogen-Air Cloud and Vaporizer Arrangement

A single vaporizer with lateral dimensions of 5 feet by 6 feet is considered for the purposes of the VCE blast load evaluation, with the flammable cloud within the vaporizer extending to a height of 9 feet (i.e., only fills a portion of the vaporizer). The volume of the congested volume filled with a hydrogen air mixture would therefore be 270 ft^3 (7.6 m^3). A flammable cloud with a length of 100 feet, a width of 50 feet, and a height of 10 feet is assumed, which gives a flammable volume of 50,000 ft^3 (1,400 m^3). This flammable cloud volume is roughly 40% that from the release scenario discussed above (i.e., this should be viewed as a relatively small cloud within the context of a typical facility explosion consequence assessment or risk analysis).

VCE blast loads (pressure and duration) were predicted using the BST method assuming a very high-speed deflagration (flame speed of Mach 1) of the flammable volume within the vaporizer (i.e., 270 ft^3) and the detonation of one-half of the flammable cloud volume (i.e., 50,000 ft^3); only one-half of the flammable cloud volume was assumed to detonate to account for a portion of the cloud being consumed as a flash fire and a portion of the cloud not participating in the detonation (i.e., due to failure of the detonation wave). The predicted VCE blast loads are shown in Figure 3. At a standoff distance greater than 100 feet (30 m), the detonation gives about 7 times the pressure and three times the duration of the deflagration, with larger blast pressure differences closer in to the vaporizer.

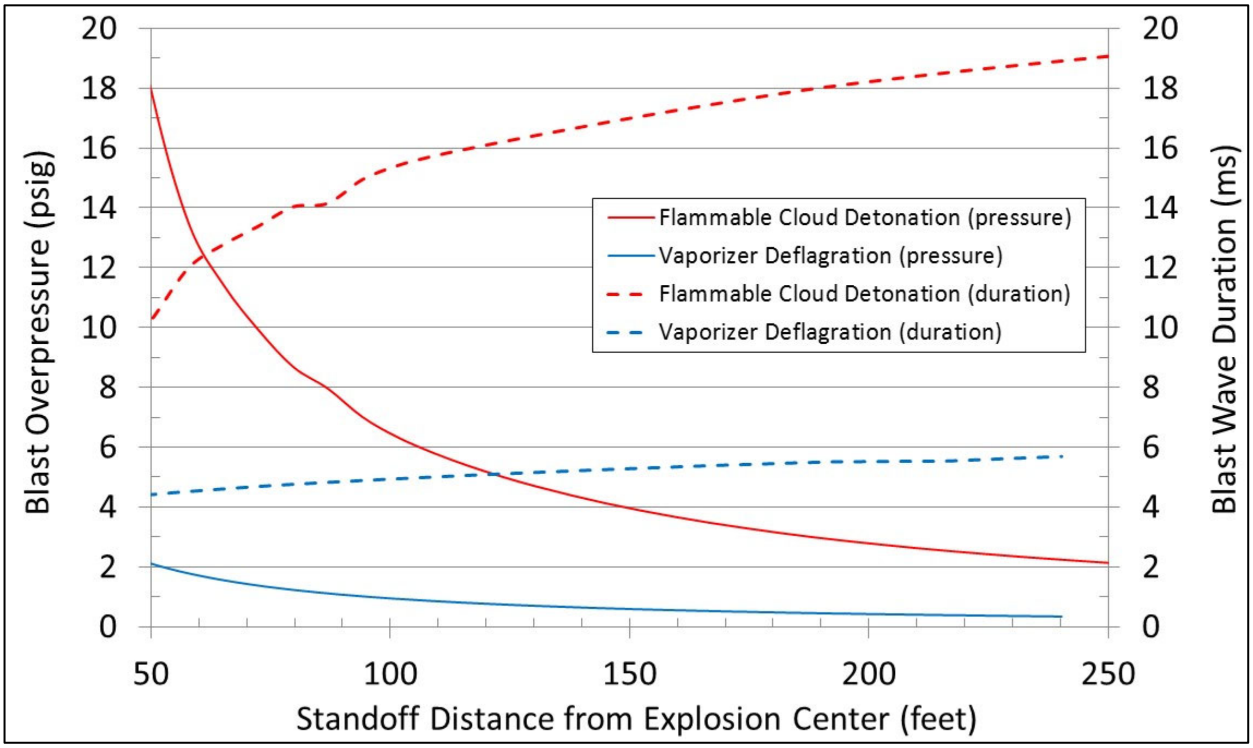

Figure 3. Blast Loads for Deflagration and Detonation of Illustrative Flammable Cloud

The resulting damage to a building can be considered to put the difference in the predicted blast loads for a deflagration and a detonation in context. The building considered for this purpose is a typical reinforced load-bearing CMU building, with the damage level predicted using BakerRisk's BEAST analysis tool [10]. Major damage and/or collapse is predicted for the detonation at a standoff distance of 150 feet, whereas only minor damage (cosmetic) is predicted for the deflagration.

This comparison illustrates the significant impact of determining whether a deflagration or a detonation occurs during a VCE involving a flammable hydrogen-air cloud engulfing an ambient vaporizer on the predicted blast loads and resulting building damage. The flammable cloud considered in this illustration is comparatively small. Larger differences between the predicted deflagration and detonation blast loads and building damage would result for a larger flammable cloud.

Vaporizer Selected for Evaluation

A “typical” vaporizer was selected for this evaluation based on field observations from range of refining and chemical processing sites. The vaporizer finned tubes have an outer diameter (OD) of 1.22 inches (3.1 cm), a fin width of 7 inches (18 cm), and a tube spacing of 12 inches (30 cm); the resulting element spacing (tip-to-tip distance) is 5.0 inches (12.7 cm). An 8×8 array was considered, giving lateral vaporizer dimensions of approximately 2.5 m. A vaporizer height of 7 m was assumed. A section of the vaporizer layout drawing is provided as Figure 4. Schematics of the vaporizer elements and element array, including key dimensions, are shown in Figure 5 and Figure 6, respectively. Example photos of a vaporizer with these design parameters are shown in Figure 7, with a close-up photo of the elements provided as Figure 8. A vaporizer based on a 6×6 array with same fin size and outer dimensions (i.e., larger tube spacing) was also evaluated in this work.

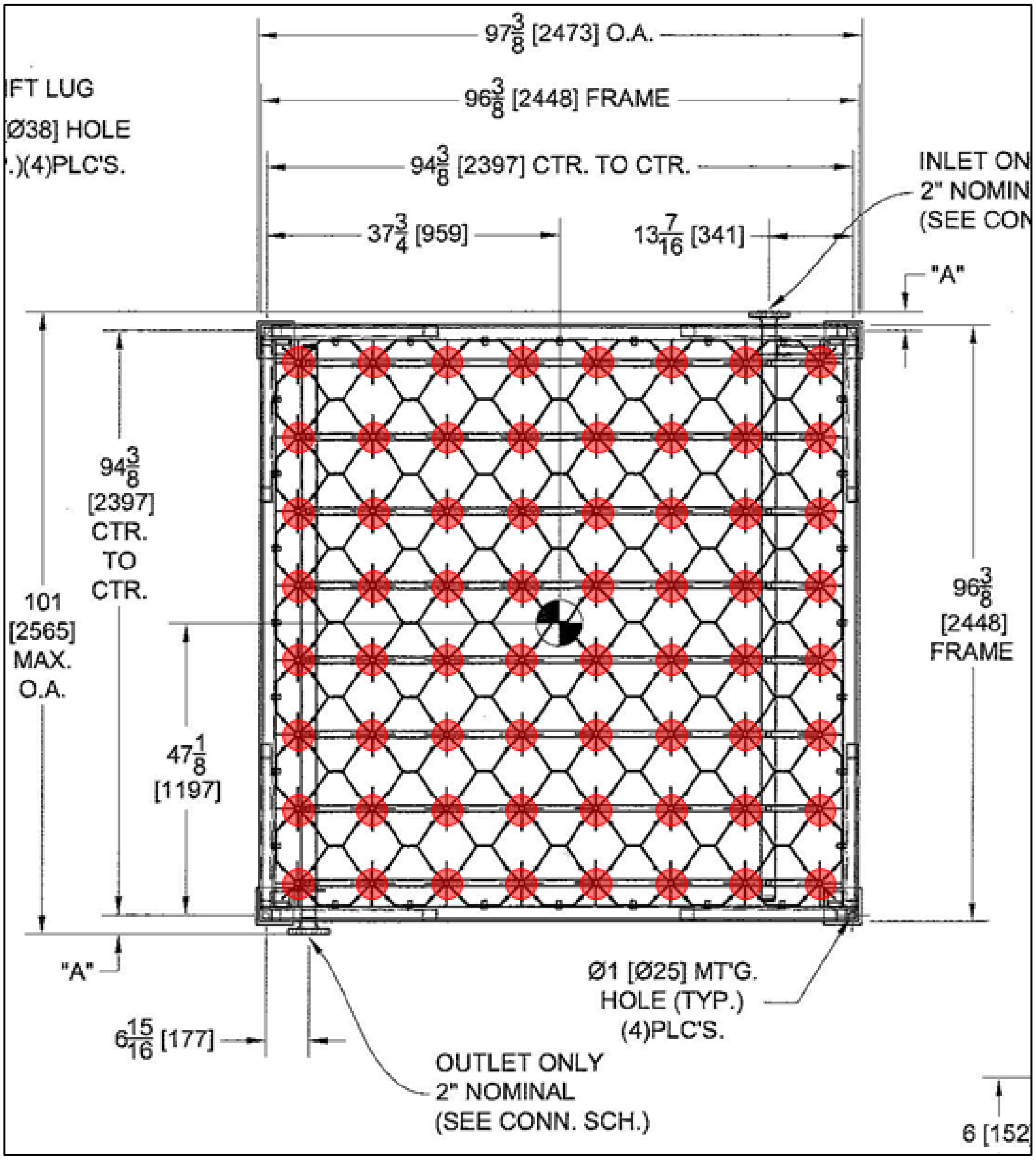

Figure 4. Vaporizer Cross Section

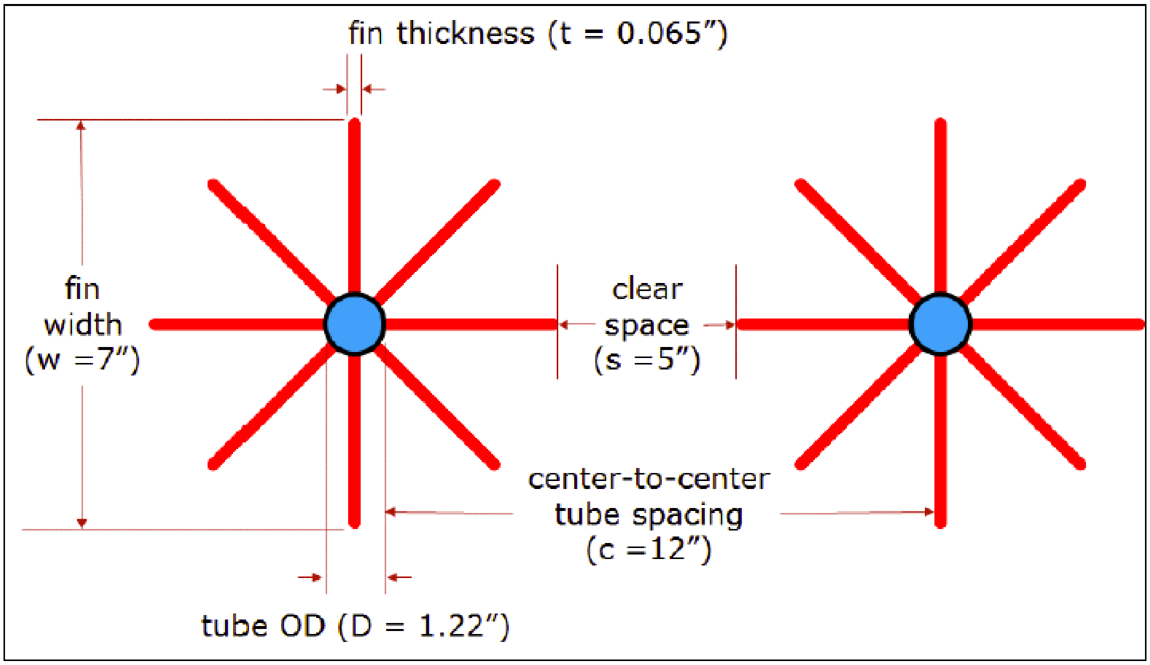

Figure 5. Vaporizer Element Schematic

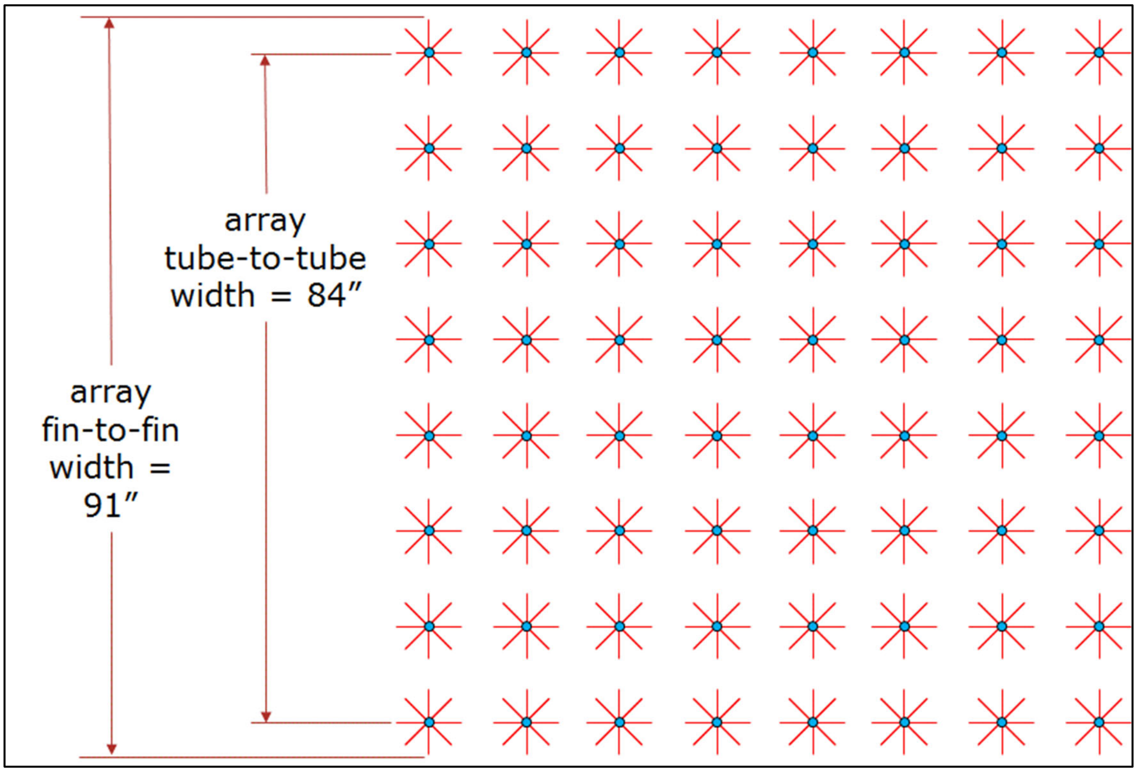

Figure 6. Vaporizer Element Array Schematic

Figure 7. Vaporizer Photographs

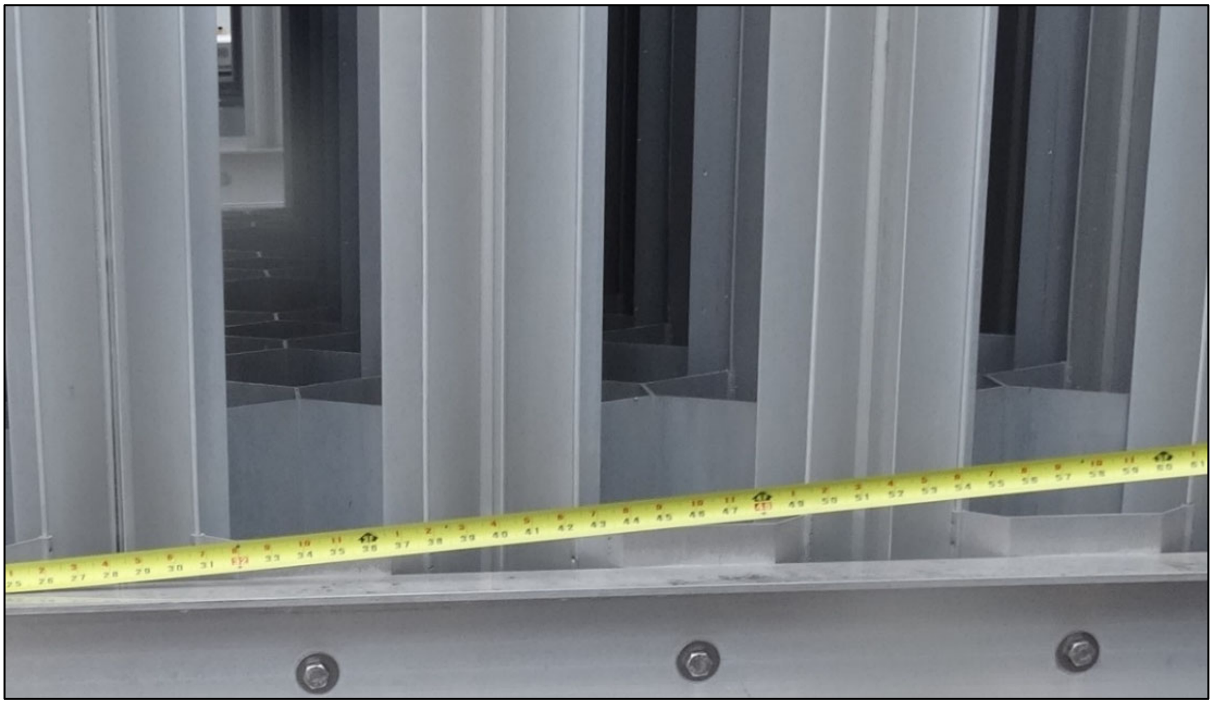

Figure 8. Photograph of Vaporizer Elements

Vaporizers are often employed in sets, with multiple vaporizers located adjacent to one another. Both a single and two-vaporizer set were evaluated in this work. A separation distance of 3 feet (1 m) was assumed, which is typical of that seen in actual installations. A separation distance of zero (i.e., a "double width" vaporizer) was also evaluated. An attempt was made to evaluate greater separation distances, but, as discussed in the results section, issues associated with the current version of FLACS precluded obtaining reliable results for vaporizer sets separated by larger distances.

FLACS Simulations

The FLACS (Flame Acceleration Simulator) CFD code was used to perform an assessment of whether a DDT would occur within a single vaporizer or a set of two adjacent vaporizers. FLACS is commonly used in industry for CFD-based dispersion and VCE simulations. FLACS solves conservation equations for mass, momentum, enthalpy, turbulence and species/combustion on a 3D Cartesian grid. Obstacles such as structural supports and pipes are represented as area porosities on control volume (CV) faces and volume porosities within a CV, with the porosity defined as the fraction of the area/volume that is available for fluid flow. The resulting porosity model is used to calculate flow resistance and turbulence source terms from objects smaller than the computational grid (i.e., subgrid), as well as the flame speed enhancement arising from flame folding.

As assessment of whether a DDT is predicted can be made using FLACS based on a combination of the dimensionless pressure gradient and normalized flame speed. The use of the dimensionless pressure gradient for this purpose was originally suggested by GexCon [11]. BakerRisk has developed both dimensionless pressure gradient and normalized flame speed criteria for FLACS assessments based on comparisons with VCE tests yielding both deflagrations and detonations.

The vaporizer design evaluated was described in the previous section. Figure 9 shows the FLACS geometry created for the simulation of a two vaporizer set. Figure 10 shows the vaporizer set engulfed in the flammable cloud along with the ignition point location. The flammable cloud was extended 2.5 m beyond the vaporizers in the short-axis direction and above the vaporizers, 5 m beyond the vaporizer nearest to the ignition source, and 0.5 m from the rear of the vaporizer opposite the ignition source. The flammable cloud was taken to be a hydrogen-air mixture at a uniform stoichiometric mixture; it should be noted that the worst-case hydrogen concentration (i.e., that most prone to a DDT) is slightly hyperstoichiometric. The ignition source was placed 1 m (3.3 ft) outside the vaporizers near grade level, such that a developed flame would propagate into the nearest vaporizer. Figure 11 shows the monitor points placed within the FLACS model to record the predicted blast pressure, pressure gradient and gas temperature history. Flame speeds were determined based on the gas temperature history (i.e., flame arrival times at monitor points).

The computational mesh was created following the guidelines in the FLACS user's manual [12], which states that, for unconfined gas clouds, that there should be a minimum of 13 grid cells across the cloud. For the smallest dimension of the vaporizer (2.5 m), this requires a computational cell size of 19 cm (i.e., 250 cm / 13). A sensitivity study was performed using a computational cell size of 15 cm, and similar results were obtained.

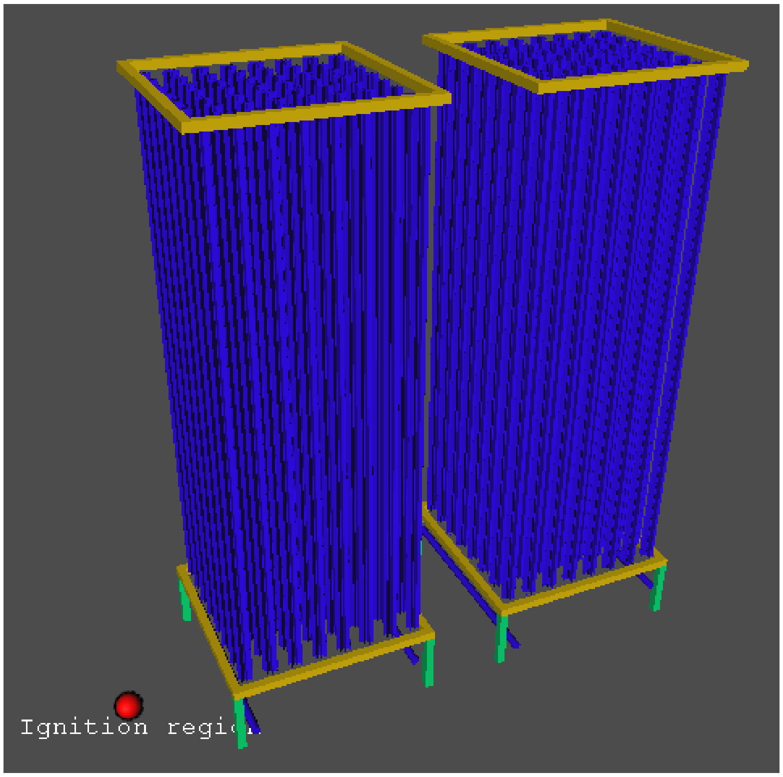

Figure 9. FLACS Solid Model of Vaporizer Pair (8×8 Array)

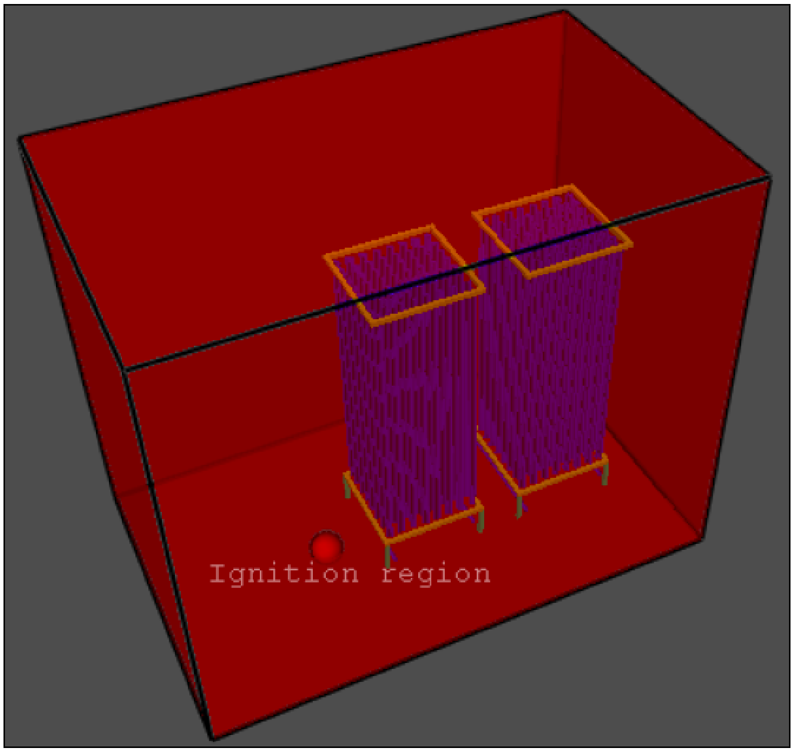

Figure 10. FLACS Model with Flammable Cloud and Ignition Point
(8×8 Array, 3-foot Separation Distance)

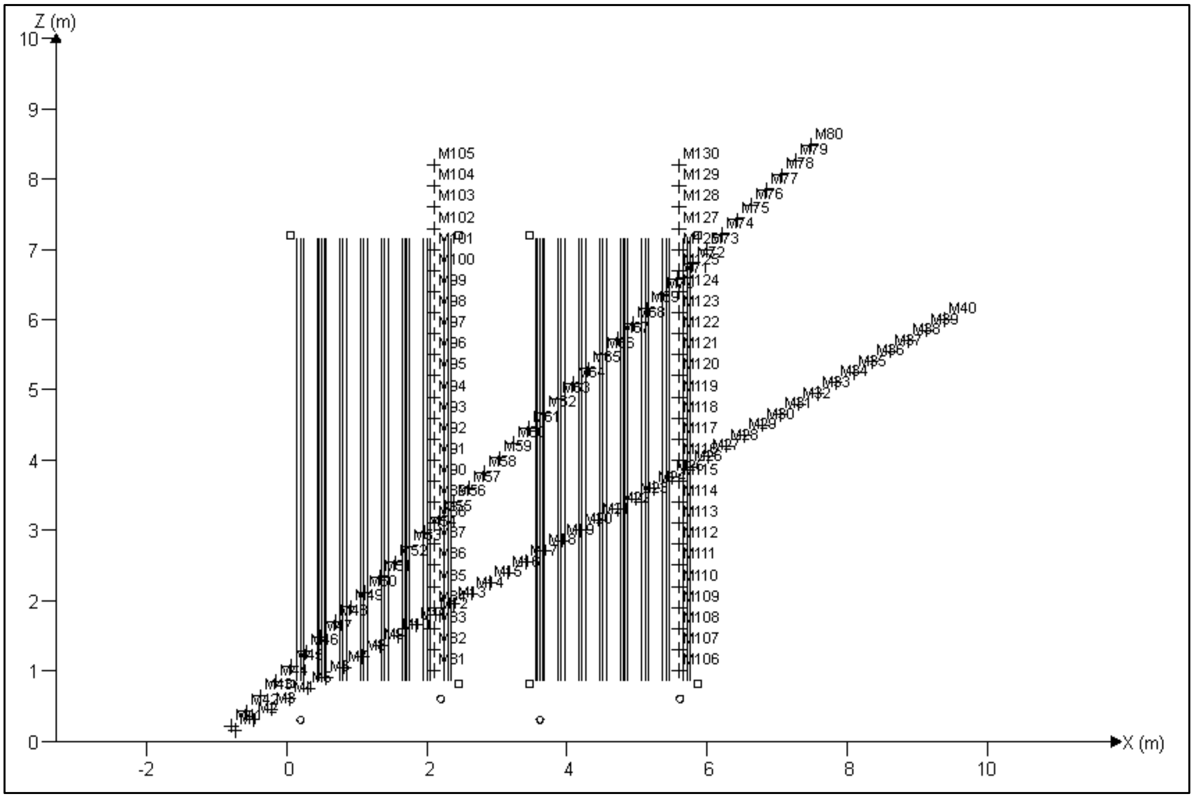

Figure 11. Target Distribution within FLACS Model

Results and Discussion

The predicted maximum dimensionless pressure gradient contour for two vaporizers with a 3-foot (1 m) separation distance between the two vaporizers is shown in Figure 12. The maximum dimensionless pressure gradient exceeds 3 over a large portion of the upper section of the second vaporizer. Dimensionless pressure gradient and normalized flame speed values along a 45-degree target line (see Figure 11) are shown in Figure 13. A DDT would be predicted based on the combination of the dimensionless pressure gradient and normalized flame speed along this target line just inside the second vaporizer. The dimensionless pressure gradient and normalized flame speed values along a 45-degree target for a set of vaporizers with no separation distance (i.e., a “double wide” vaporizer) are shown in Figure 14; a DDT would once again be predicted along this target line just inside the second vaporizer.

Analyses were also performed at lean (23%H_2, 0.71 ER) and rich (35%H_2, 1.28 ER) fuel concentrations. Both 8×8 and 6×6 vaporizer arrays were evaluated, assuming no separation distance between two adjacent vaporizers. The results are shown in Table 1. For the 8×8 array set, DDTs were predicted for all three fuel concentrations examined, with the flame travel distance required for a DDT decreasing slightly with the rich fuel concentration. For the 6×6 array, a DDT was not predicted for the lean fuel concentration, and the flame travel distance required for a DDT decreasing slightly with the rich fuel concentration.

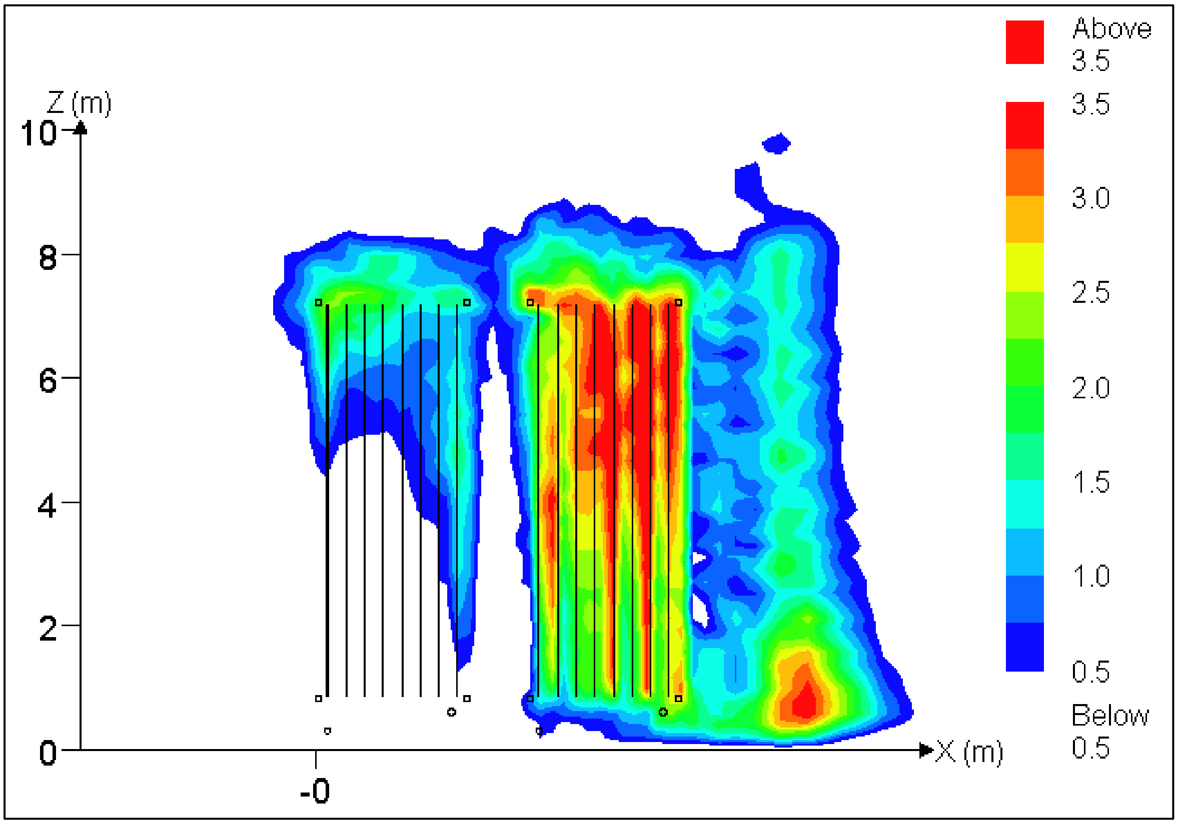

Figure 12. Maximum Dimensionless Pressure Gradient Contour (1 m separation distance)

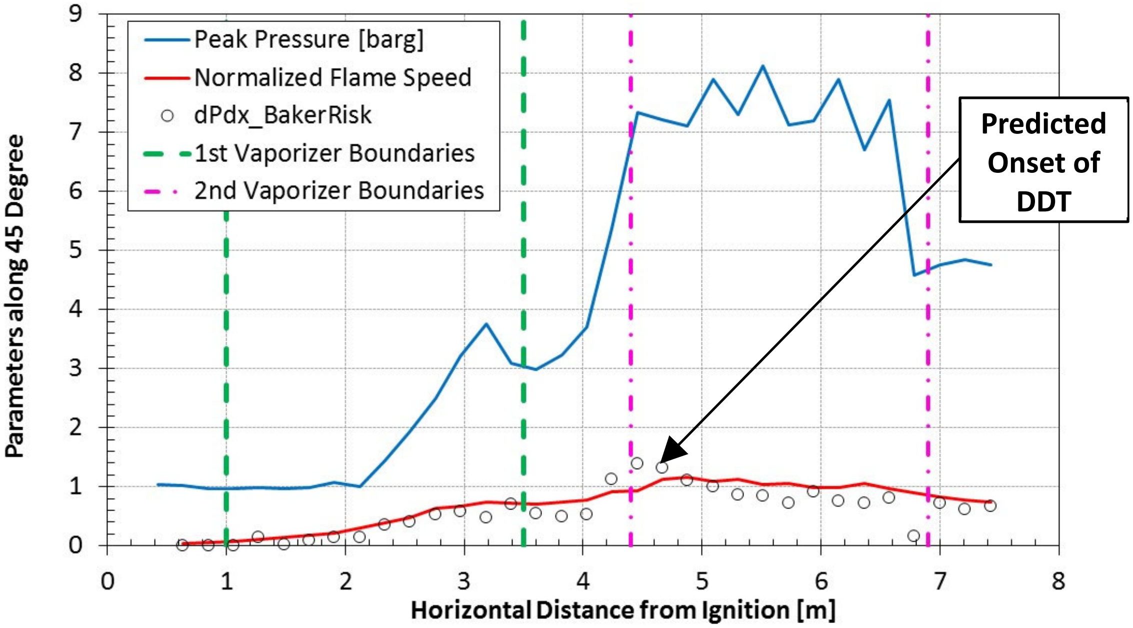

Figure 13. Maximum Dimensionless Pressure Gradient and Normalized Flame Speed
(45-degree target line, 1 m separation distance between vaporizers)

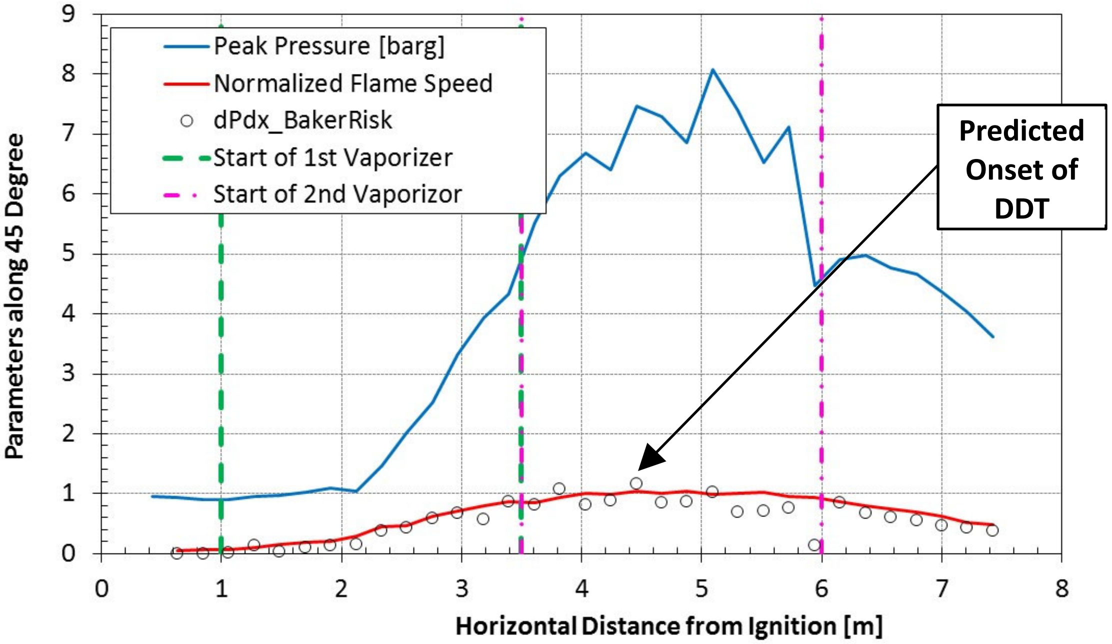

Figure 14. Maximum Dimensionless Pressure Gradient and Normalized Flame Speed (45-degree target line, no separation between vaporizers)

Table 1. Horizontal Distance for DDT with Adjoined Vaporizer Arrays

Vaporizer Array (two adjacent vaporizers)	**Separation Distance (feet)**	**DDT Location (m) for Specified Hydrogen Concentration (equivalence ratio / % hydrogen)**		
		0.7 (23%)	**1 (30%)**	**1.3 (35%)**
8×8	0	3.5 m	3.5 m	3.2 m
6×6	0	-	3.5 m	3.2 m

Issues with the ability of FLACS to accurately predict flame acceleration in a second congested volume (i.e., where two adjacent congested volumes are separated by some distance) has been reported in the literature [13], where the underlying issue was identified to be the turbulent length scale assigned by FLACS; it was determined that this issue would impact FLACS simulations where the second congested volume was separated by one to times the size of the congested volumes (i.e., by approximately 8 feet or more for the vaporizers considered in this work). A potential approach (i.e., "data dump technique") was identified [13], but this approach was not deemed to be applicable to the current analysis. Furthermore, the data dump technique was "only a suggestion for others working in this area" rather than an approach which had been thoroughly tested or which was ready for incorporation into FLACS. The FLACS developer (i.e., GexCon) is aware of this issue and is actively working to resolve it. A joint industry project (MEASURE) may develop information which could help address this issue.

Conclusions and Recommendations for Future Work

The results of this analysis indicate that a DDT would not occur for a single vaporizer of the type evaluated, even for worst-case hydrogen-air mixtures. It should be noted that this analysis implicitly assumes that a single vaporizer would be located well away from other congested volumes. A single vaporizer with significantly larger dimensions and/or tighter element spacing could potentially result in the prediction of a DDT.

A DDT would be expected based on the results of this analysis for a pair of closely-spaced (i.e., 3 foot separation distance) 8×8 vaporizers for all hydrogen concentrations evaluated (i.e., 23%H_2 to 35%H_2). The DDT was predicted to occur approximately ½ meter inside the second vaporizer (i.e., shortly after the flame enters the second vaporizer). As discussed earlier, a detonation, once triggered by a DDT within a vaporizer, could propagate through a significant portion of the remaining flammable cloud, which could extend well beyond the vaporizer set. A DDT would not be expected for smaller vaporizers at lean hydrogen concentrations (e.g., a 6×6 array at 23%H_2). It should be recognized that a flammable hydrogen-air cloud engulfing a set of vaporizers from an actual release may not trigger a DDT due to the hydrogen concentration at the vaporizer set (i.e., may be too lean or too rich).

It is recommended that this CFD analysis be revisited when a version of FLACS is released that addresses the issues associated with predicting the flame acceleration in a second congested volume. As discussed earlier, this is a known issue that is currently being addressed by the code developer. The extended CFD analysis should include an evaluation of the impact of vaporizer design parameters (array size, element spacing, etc.), as well as vaporizer separation distance. Air Liquide has performed additional analyses which indicate the effect of the hydrogen-air mixture temperature is relevant, with lower temperatures expected to give slightly less flame acceleration and decrease the potential for a DDT.

It is also recommended that explosion tests be performed with hydrogen-air mixtures engulfing both single vaporizers and vaporizer sets in order to provide definitive benchmark data. Benchmark data for this type of congested volume is important to validate the CFD predictions, particularly for establishing the separation distance required to preclude a DDT. Such tests could include the effect of an actual release versus a premixed hydrogen-air cloud.

References

---

1 Thomas, J.K., C.D. Eastwood and M.L. Goodrich (2015) “Are Unconfined Hydrogen Vapor Cloud Explosions Credible?” Process Safety Progress, 34(1): 36-43

2 Baker, Q.A. et al. (2010) Guidelines for Vapor Cloud Explosion, Pressure Vessel Burst, BLEVE and Flash Fire Hazards, Second Edition, Center for Chemical Process Safety (CCPS) & John Wiley and Sons, New York, NY.

3 Pierorazio, A.J., J.K. Thomas, Q.A. Baker and D.E. Ketchum (2005) “An Update to the Baker-Strehlow-Tang Vapor Cloud Explosion Prediction Methodology Flame Speed Table,” Process Safety Progress, 24(1): 59-65.

4 Thomas, J.K., A.J. Pierorazio, M. Goodrich, M. Kolbe, Q.A. Baker and D.E. Ketchum (2003) “Deflagration to Detonation Transition in Unconfined Vapor Cloud Explosions,” Center for Chemical Process Safety (CCPS) 18th Annual International Conference & Workshop, Scottsdale, AZ, 23-25 September 2003.

5 Thomas, J.K., R.J. Duran and M.L. Goodrich (2010) “Deflagration to Detonation Transition in a Lean Hydrogen-Air Unconfined Vapor Cloud Explosion,” Mary Kay O’Connor Process Safety International Symposium,” College Station, TX, October 27, 2010.

6 Thomas, J.K. and D.R. Malik (2017) “Ammonia and Hydrogen Vapor Cloud Explosion Testing (A Tale of Two Gases),” 62nd Annual Safety in Ammonia Plants and Related Facilities Symposium, New York, September 10-14, 2017.

7 Royle, M, Shirvill, LC and Roberts, TA, “Vapour Cloud Explosion from the Ignition of Methane/Hydrogen/Air Mixtures in Congested Region. http://ukelg.ps.ic.ac.uk/40GC1.pdf.

8 Thomas, J.K., M.L. Goodrich and R.J. Duran (2013) “Propagation of a Vapor Cloud Detonation from a Congested Area into an Uncongested Area: Demonstration Test and Impact on Blast Load Prediction,” Process Safety Progress, 32(2): 199-206.

9 Duran, R.J., M.L. Goodrich and J.K. Thomas (2012) “Propagation of a Vapor Cloud Detonation from a Congested into an Uncongested Area,” Chem. Eng. Trans., Vol. 26.

10 BEAST (building assessment tool developed by BakerRisk for the Explosion Research Cooperative Joint Industry Program).

11 Middha, P. and O.R. Hansen (2008) “Predicting Deflagration to Detonation Transition in Hydrogen Explosions,” Process Safety Progress, 27)3): 192-204.

12 Gexcon AS, “FLACS Version 10.5 User’s Manual,” 5/27/16.

13 Ma, G., J. Li and M. Abdel-Jawad (2014) “Accuracy Improvement in Evaluation of Gas Explosion Overpressures in Congestions with Safety Gaps,” J. Loss Prev. in the Process Ind., 32: 358-66.