# VALIDATION OF THE MAIN CONSEQUENCE MODELLING PARAMETERS OBTAINED WITH HAMS ADVANCED QUANTITATIVE RISK ASSESSMENT SOFTWARE IN COMPARISON WITH SIMILAR ALOHA AND CCPS SOFTWARE

#### 1. Introduction

HAMSAGARS is an Indian company which developed advanced research and software development capabilities since 2001, based on safety audits, quantitative risk assessment studies, process safety reviews, job safety analysis, and modeling for environmental impact assessments.

HAMSAGARS owns advanced software applications for gas plume dispersion modeling, thermal radiation from fires, and overpressure shock waves from explosions, which facilitates the calculation of societal and individual risk in hazardous industries. The company provides software models to the fertilizer, pharmaceutical, petrochemical, and heavy chemical industries. The HAMSAGARS quantitative risk assessment (QRA) software (HAMS) is applied by more than 85 companies in these industries.

The software package of the company is called HAMS-GPS PSM/EHS Management Software for Advanced Quantitative Risk Assessment (QRA), Consequence Risk Analysis for Societal and Individual Risk.

Validation of QRA software by the suppliers is not an easy task. If it involves the measurement of consequence model outcomes with actual catastrophic results, the process becomes shaky due to the many interdependent and independent variables that play a role and the reliability of evidence data that is available afterwards.

In order to validate the outcomes of the HAMS software package, the consequence results obtained with the software were compared with the results from the following software packages that are applied internationally for many years:

- US Environmental Protection Agency. US National Oceanic and Atmospheric Administration. US Chemical Emergency Preparedness and Prevention Office. US Hazardous Materials Response Division. Computer-aided Management of Emergency Operations used in conjunction with the Areal Locations of Hazardous Atmospheres (ALOHA). This software is used by more than 40 countries in the world and was validated through international peer review, for example to analyse the Somerset West sulphur fire of 1997.
- American Institute of Chemical Engineers (AIChE). Center for Chemical Process Safety (<u>CCPS</u>). Guidelines for Chemical Process Quantitative Risk Analysis. Second Edition. The software packages developed by scientists, engineers and risk assessors over the world are based on continuous research of the fundamental mathematical equations which are used in all quantitative risk assessment software from all suppliers.

#### 2. Objective of the study

Any computer software programme needs to be validated to confirm that the requirements for its specific intended use or application have been fulfilled. This is prescribed in the ISO/IEC/IEEE-12207 Standard: Systems and Software Engineering – Software Life Cycle Processes. The objective of this study is to validate the HAMS software against known, validated international software packages with regard to consequence modelling for fires, vapour cloud explosions and toxic gas dispersion.

#### 3. Methodology

Three hypothetical scenarios were formulated for analysis with the three software packages, ALOHA, CCPS and HAMS. These scenarios covered a fire, vapour cloud explosion and the dispersion of a toxic gas. Details are as follows:

- <u>Scenario 1</u>. An LPG storage tank aboveground; 22 500-liters; 7-barg; thermal radiation flux from a BLEVE at 37.5 kW/m2.
- <u>Scenario 2</u>: An LPG storage tank aboveground; 22 500-liters; 7-barg; 25-mm hole leak for 60 minutes; shock wave overpressure of 5 psi.
- <u>Scenario 3</u>: A chlorine storage tank of 925-kg; uncontrolled release opening of 25-mm for 60-minutes; ERPG-3 criterion of 20-ppm; wind direction east at 3 m/s; urban conditions; Pasquill stability class F; 50% humidity; ambient temperature 25 °C.

Three comparative evaluations were done on the consequence outcomes of the software packages, using the ALOHA, CCPS and HAMS software packages as follows:

- CCPS versus ALOHA.
- HAMS versus ALOHA.
- HAMS versus CCPS.

#### 4. Validation model runs

The outcome of the various model simulations are shown in Appendices A to C.

## 1. Validation scenario 1: BLEVE

Table 1: Consequence modelling results for BLEVE

Modelling parameters	S	LOHA oftware neters	CCPS software meters	HAMS software meters
LPG tank aboveground; 22 500-liters; 7-thermal radiation flux of 37.5 kW/m2	-barg;	143	94	81

## 2. Validation scenario 2: Vapour cloud explosion (VCE)

Table 2: Consequence modelling results for VCE

Modelling parameters	ALOHA	CCPS	HAMS
	software	software	software
	meters	meters	meters
LPG tank aboveground; 22 500-liters; 7-barg; 25-mm hole leak for 60 minutes; shock wave overpressure of 5 psi	40	56	27

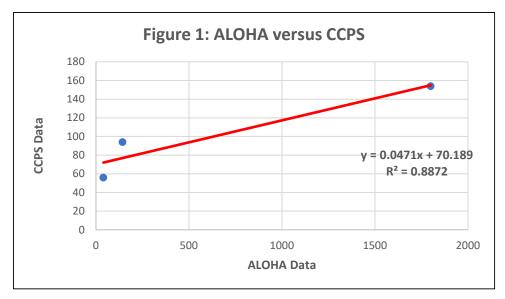
## 3. Validation scenario 3: Release of toxic chlorine

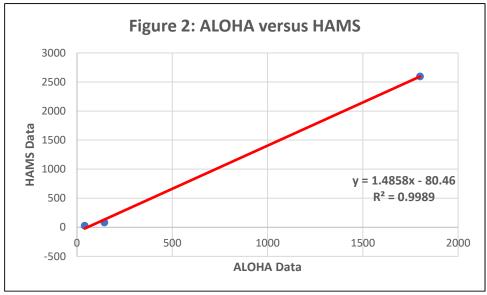
Table 3: Consequence modelling results for toxic gas dispersion

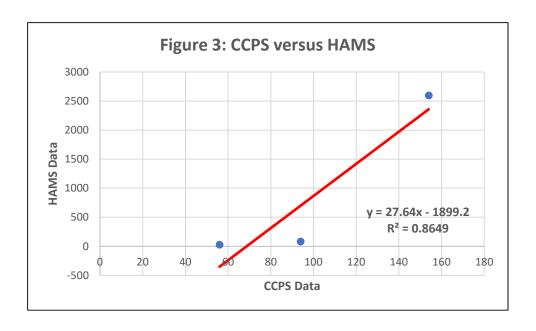
Modelling parameters	ALOHA	CCPS	HAMS
	software	software	software
	meters	meters	meters
Storage tank of 925-kg; uncontrolled release opening of 25-mm for 60-minutes; ERPG-3 criterion of 20-ppm; wind direction east at 3 m/s; urban conditions; Pasquill stability class F; 50% humidity; ambient temperature 25 °C	1 800	154	2 597

#### 4. Comparison of the results

An appropriate statistical test, namely R<sup>2</sup> (coefficient of determination or correlation coefficient) was applied. This statistical test describes the proportion of the variation in the dependent parameter that is predicted by the independent variable. In this study the outcomes of the ALOHA and CCPS software acted as independent variables respectively, while the HAMS software outcomes acted as dependent variables. The three comparative evaluations are shown in the following graphs (Figures 1 to 3):







#### 5. Conclusions

The outcomes of the three software packages for a BLEVE lie within an acceptable range, between 81 and 143 meters. The outcomes for a VCE lie within an acceptable range, between 27 and 65 meters. The outcomes for chlorine gas dispersion vary significantly between tween 154 and 2 597 meters. The ALOHA software is known for its conservative estimation of toxic gas plume dispersion.

The coefficients of determination ( $R^2$ ) were determined for each data set comparison. In this study, the dependent variable was the HAMS consequence outcome, while the independent variables were the ALOHA and CCPS consequence outcomes respectively. The  $R^2$  values were as follows:

- CCPS versus ALOHA: R<sup>2</sup> = 89%.
- HAMS versus ALOHA: R<sup>2</sup> = 99%.
- HAMS versus CCPS: R<sup>2</sup> = 86%.

These results showed that the consequence model outcomes of the HAMS software compares favourably with the international ALOHA and CCPS software packages. In general science and engineering, an R<sup>2</sup> value of 60% is considered significant. In all three comparisons, this level was exceeded.

#### 6. Level of uncertainty

According to research done by the Center for Chemical Process Safety (CCPS) of the American Institute of Chemical Engineers (AIChE) the results of quantitative risk assessment consequence modelling, using different mathematical models, may differ by a factor as high as 5, for example between the solid plume model and the point source model for the estimation of the radiation from a burning pool.

#### 7. Requirements for validation specified by ISO/IEC/IEEE-12207

Section 3.1.71 of the abovementioned international Standard defines "validation" as confirmation, through the provision of objective evidence, that the software requirements for a specific intended use or application have been fulfilled. The standard further prescribes that software validation methods must include the following:

- Inspection.
- Analysis.
- Analogy/similarity.
- Demonstration.
- Simulation.
- · Peer review.
- Testing.

The validation technique applied in this report is based on analogy and similarity between HAMS, ALOHA and CCPS.

#### 8. References

- US Environmental Protection Agency. US National Oceanic and Atmospheric Administration. US Chemical Emergency Preparedness and Prevention Office. US Hazardous Materials Response Division. Computer-aided Management of Emergency Operations used in conjunction with the Areal Locations of Hazardous Atmospheres (ALOHA).
- American Institute of Chemical Engineers (AIChE). Center for Chemical Process Safety (CCPS). Guidelines for Chemical Process Quantitative Risk Analysis. Second Edition.

- HAMS-GPS PSM/EHS Management Software for Quantitative Risk Assessment (QRA), Consequence Risk Analysis for Societal and Individual Risk.
- ISO/IEC/IEEE-12207: Systems and Software Engineering Software Life Cycle Processes.

#### Report compiled by:

Dr Alfonso Niemand BSc; MBL; PhD

Date: 30 December 2022

Declaration of independence and objectivity:

I, Alfonso Niemand, declare that I have compiled this validation report independently and objectively and that I have no relation, other than a software user, with the company HAMSAGARS who is the supplier of the HAMS-GPS PSM/EHS Management Software for Advanced Quantitative Risk Assessment (QRA), Consequence Risk Analysis for Societal and Individual Risk.

## Appendix A: CCPS model output

## Validation scenario 1: BLEVE

## **Cross-correlation 2.27: BLEVE Thermal Flux**

Input Data:					
Initial flammable	mass:		22500	Liters	
Initial flammable	mass:		12375	kg	<30 000
Water partial pre	ssure in air:		2810	Pascal	
Radiation Fraction	n, R		0.3		
Distance from fire	eball centre on g	round:	93.5	m	
Heat of Combusti	on of fuel:		50368	kJ/kg	
Density of liquid:			0.55	kg/l	
Calculated					
Results:					
Maximum firebal	l diameter:		134.2	m	
Fireball combusti	on duration:		10.4	S	
Centre height of f	fireball:		100.6	m	
Initial ground leve	el hemisphere di	ameter:	174.4	m	
Surface emitted f	lux:		317.9	kW/m**2	•
Path length:			70.3		
Transmissivity:			0.674		
Surface area of e	mitter		95594.04	m2	
	Horizontal	Vertical	<u> </u>		
View Factor:	0.17	0.16			
Received flux:	37.44	34.79	kW/m**2		

## Validation scenario 2: Vapour cloud explosion (VCE)

#### Cross-correlation 2.4: Gas Discharge through a Hole

Input [	Data:
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Heat capacity ratio of gas:	1.15	
Hole size:	25	mm
Upstream pressure:	7	bar abs
Downstream pressure:	1.01	bar abs
Temperature:	298	K
Gas molecular weight:	51	

#### Excess Head Loss Factors:

Entrance:		0.5
Exit:		1
Others:		0
	TOTAL:	1.5

#### Calculated Results:

Hole area:	0.000490874	m**2
Upstream gas density:	14.41	kg/m**3
Expansion factor, Y:	0.614	

Actual pressure ratio: 0.86

Heat capacity ratio, k:	1.2	1.4	1.67	_
Sonic pressure ratios:	0.536	0.575	0.618	
Choked pressure:	3.25	2.98	2.68	bar
Mass flow:	0.8096	0.8384	0.8693	kg/s

Interpolation table: 1.2 0.809567448 1.4 0.838440173

0.802340 kg

Interpolated	d mass flow:	0.802349	kg/s
Gas releas	e in 60 minutes	2888.5	kg
Gas releas	e in 10 minutes	481.4	kg

## Cross-correlation 2.20: TNT Equivalency of a Vapour Cloud

Explosion overpressure yield	0.03	%
Mass of gas	2888.5	kg
Higher heating value of cloud	50000	kJ/kg
Higher heating value of TNT	4652	kJ/kg

Liquid volume of gas: Equivalent

mass

TNT

Density of liquid:

######## 0.74

liters

kg kg/l

Input Data:

TNT Mass: 931 Distance from blast: 56

Calculated Results:

Scaled distance, z: m/kg\*\*(1/3) 5.7343

Overpressure Calculation: (only valid for z > 0.0674 and z < 40)

kg

m

a+b\*log(z): 0.809845

Overpressure: 34.20 kPa

> 4.961946 psig

Impulse Calculation: (only valid for z > 0.0674 and z < 40)

a+b\*log(z): -0.12144

Impulse: 52.37476 Pa s

**Duration Calculation:** (only valid for z > 0.178 and z < 40)

a+b\*log(z): -0.90927

Duration: 3.984263 ms

Arrival Time Calculation: (only valid for z > 0.0674 and z < 40)

a+b\*log(z): 0.84264

Arrival time: 10.135 ms

## Validation scenario 3: Release of toxic chlorine

Example 2.13: Plume Release #1

Input Data:			
Release rate:	0.1	kg/s	
Molecular weight:	35.5		
Temperature:	298	K	
Pressure:	2	atm	
Release height:	0	m	
Distance downwind:	154	m	< X
Distance off wind:	0	m	< Y
Distance above ground:	1	m	< Z
Calculated Results:			

#### **RURAL CONDITIONS:**

	********		Stability Classes **********************************				
	A	В	С	D	E	F	_
Assumed wind speed:	0.1	0.1	2	3	2	2	m/s
Dispersion Coefficients:							
Sigma y:	33.62	24.45	16.81	12.23	9.17	6.11	m
Sigma z:	30.80	18.48	12.13	8.33	4.42	2.36	m
		7.03E-	7.78E-	1.03E-	3.83E-	1.01E-	
Downwind concentration:	3.07E-04	04	05	04	04	03	kg/m**3
	307.22	703.38	77.75	103.46	383.09	1010.15	mg/m**3
PPM:	105.81	242.26	26.78	35.63	131.95	347.92	PPM

#### **URBAN CONDITIONS:**

	********* Stability Classes **********				
	A-B	С	D	E-F	_
Assumed wind speed:	0.1	2	3	3	m/s
Dispersion Coefficients:					
Sigma y:	47.83	32.88	23.91	16.44	m
Sigma z:	39.70	30.80 1.57E-	17.83 2.48E-	11.10 5.79E-	m
Downwind concentration:	1.68E-04	05	05	05	kg/m**3
	167.57	15.71	24.84	57.88	mg/m**3
PPM:	57.71	5.41	8.56	19.94	PPM

#### Appendix B: ALOHA model output

Validation scenario 1: BLEVE

#### SITE DATA:

Location: VALIDATION, SOUTH AFRICA

Building Air Exchanges Per Hour: 0.62 (unsheltered single storied)

#### **CHEMICAL DATA:**

Chemical Name: PROPANE

CAS Number: 74-98-6 Molecular Weight: 44.10 g/mol

ERPG-1 (60 min): 5500 ppm ERPG-2 (60 min): 17000 ppm ERPG-3 (60 min): 33000

ppm

IDLH: 2100 ppm LEL: 21000 ppm UEL: 95000 ppm

Ambient Boiling Point: -46.1° C

Vapor Pressure at Ambient Temperature: greater than 1 atm

Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

#### ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)

Wind: 3 meters/second from E at 3 meters

Ground Roughness: urban or forest Cloud Cover: 5 tenths

Air Temperature: 25° C

Stability Class: F (user override)

No Inversion Height Relative Humidity: 50%

#### SOURCE STRENGTH:

BLEVE of flammable liquid in horizontal cylindrical tank

Tank Diameter: 2 meters Tank Length: 7.16 meters

Tank Volume: 22500 liters

Tank contains liquid

Internal Storage Temperature: 25° C

Chemical Mass in Tank: 11,048 kilograms

Tank is 100% full

Percentage of Tank Mass in Fireball: 100%

Fireball Diameter: 129 meters Burn Duration: 9 seconds

#### THREAT ZONE:

Threat Modeled: Thermal radiation from fireball

Red: 143 meters --- (37.5 kW/(sq m))

Orange: 416 meters --- (5.0 kW/(sq m) = 2nd degree burns within 60 sec)

Yellow: 648 meters --- (2.0 kW/(sq m) = pain within 60 sec)

#### Validation scenario 2: Vapour cloud explosion (VCE)

#### SITE DATA:

Location: VALIDATION, SOUTH AFRICA

Building Air Exchanges Per Hour: 0.62 (unsheltered single storied)

#### **CHEMICAL DATA:**

Chemical Name: PROPANE

CAS Number: 74-98-6 Molecular Weight: 44.10 g/mol

ERPG-1 (60 min): 5500 ppm ERPG-2 (60 min): 17000 ppm ERPG-3 (60 min): 33000

ppm

IDLH: 2100 ppm LEL: 21000 ppm UEL: 95000 ppm

Ambient Boiling Point: -46.1° C

Vapor Pressure at Ambient Temperature: greater than 1 atm

Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

#### ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)

Wind: 3 meters/second from E at 3 meters

Ground Roughness: urban or forest Cloud Cover: 5 tenths

Air Temperature: 25° C

Stability Class: F (user override)

No Inversion Height Relative Humidity: 50%

#### SOURCE STRENGTH:

Leak from hole in horizontal cylindrical tank

Flammable chemical escaping from tank (not burning)

Tank Diameter: 2 meters Tank Length: 7.16 meters

Tank Volume: 22500 liters

Tank contains liquid Internal Temperature: 25° C

Chemical Mass in Tank: 11,048 kilograms

Tank is 100% full

Circular Opening Diameter: 2.5 centimeters

Opening is 10 centimeters from tank bottom

Release Duration: 24 minutes

Max Average Sustained Release Rate: 520 kilograms/min

(averaged over a minute or more)

Total Amount Released: 11,048 kilograms

Note: The chemical escaped as a mixture of gas and aerosol (two phase flow).

#### THREAT ZONE:

Threat Modeled: Overpressure (blast force) from vapor cloud explosion

Type of Ignition: ignited by spark or flame

Level of Congestion: congested

Model Run: Heavy Gas

Red: 40 meters --- (5 psi)

Orange: 47 meters --- (3.5 psi = serious injury likely)

Yellow: 97 meters --- (1.0 psi = shatters glass)

#### Validation scenario 3: Release of toxic chlorine

#### SITE DATA:

Location: VALIDATION, SOUTH AFRICA

Building Air Exchanges Per Hour: 0.62 (unsheltered single storied)

#### CHEMICAL DATA:

Chemical Name: CHLORINE

CAS Number: 7782-50-5 Molecular Weight: 70.91 g/mol

ERPG-1 (60 min): 0.5 ppm ERPG-2 (60 min): 2 ppm ERPG-3 (60 min): 20 ppm

IDLH: 10 ppm

Ambient Boiling Point: -38.0° C

Vapor Pressure at Ambient Temperature: greater than 1 atm

Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

#### ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)

Wind: 3 meters/second from E at 3 meters

Ground Roughness: urban or forest Cloud Cover: 5 tenths

Air Temperature: 25° C

Stability Class: F (user override)

No Inversion Height Relative Humidity: 50%

#### SOURCE STRENGTH:

Leak from hole in horizontal cylindrical tank

Non-flammable chemical is escaping from tank

Tank Diameter: 0.8 meters Tank Length: 1.4 meters

Tank Volume: 704 liters

Tank contains liquid Internal Temperature: 25° C

Chemical Mass in Tank: 925 kilograms

Tank is 94% full

Circular Opening Diameter: 2.5 centimeters

Opening is 10 centimeters from tank bottom

Release Duration: 2 minutes

Max Average Sustained Release Rate: 759 kilograms/min

(averaged over a minute or more)

Total Amount Released: 882 kilograms

Note: The chemical escaped as a mixture of gas and aerosol (two phase flow).

#### THREAT ZONE:

Model Run: Heavy Gas

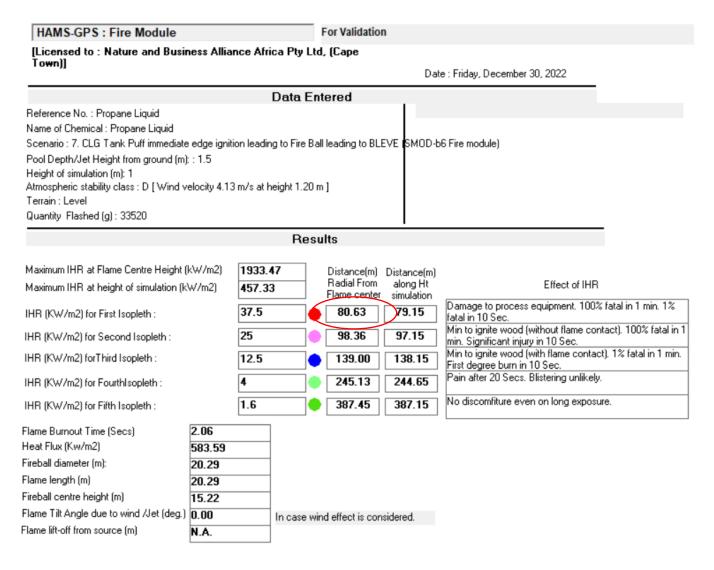
Red : 1.8 kilometers --- (20 ppm = ERPG-3)

Orange: 4.4 kilometers --- (3 ppm = ERPG-2)

Yellow: 7.3 kilometers --- (1 ppm = ERPG-1)

#### **Appendix C: HAMS model output**

#### Validation scenario 1: BLEVE



\* IHR - Intensity of Heat / Thermal Radiation

NOTE: Without wind effect considered for computing Radial distance, distance along Ht. and other results.

#### Validation scenario 2: Vapour cloud explosion (VCE)

For Validation HAMS-GPS: Explosion Module

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Date: Friday, December 30, 2022

#### Data Entered

Reference No.: Propane Liquid Name of Chemical: Propane Liquid

Scenario : 6. CLG Gas Main Pipe leak Gas delayed internal ignition leading to Explosion scenario (UCE module)

Cloud height at Pool/Dyke Depth from ground (m): : 1.00

Height of simulation (m): 1

TNT Equivalent of the chemical:: 2 Explosion Mass (lbm): 2447 Explosion Type: Unconfined explosion

#### Results

#### Explosion Summary at Height of simulation (m) 1.00

- 1, Cloud Radius (m): 5.28
- 2. Explosion Yield Factor: 0.61
- 1. Storage tank/frameless structure damage limit (m): 38.89 [ psi : 3.00 , Bar : 0.2069 ]
- 2. 50% BrickWall damage 4-9 inch thick distance limit (m): 46.42 [ psi : 2.50 , Bar : 0.1725 ] 3. Sheet/Panel damage 3 mm thick limit (m): 121.28 [ psi : 1.00 , Bar : 0.0689 ]
- 4. Safe distance/Missile limit (m): 469.00 [ psi : 0.40 , Bar : 0.0276 ]
- 5. 100% Fatal distance (m): 11.46 [ psi : 30.77 , Bar : 2.1213 ]
- 6. 50% Fatal distance (m): 14.39 [ psi : 17.93 , Bar : 1.2360 ] 7. Fatal distance limit (m): 19.39 [ psi : 8.81 , Bar : 0.6076 ]
- 8. 100% Structural damage limit (m): 21.95 [ psi : 6.56 , Bar : 0.4520 ] 9. 50% Structural damage limit (m): 62.88 [ psi : 1.83 , Bar : 0.1261 ]
- 10. Structural damage limit (m): 158.01 [ psi : 0.82 , Bar : 0.0564 ]
- 11. Ear drum injuries limit (m): 163.43 [ psi : 0.80 , Bar : 0.0550 ]
- 12. 100% Glass break 3-5 mm thick limit (m): 81.69 [ psi : 1.40 , Bar : 0.0963 ]
- 13. 50% Glass break 3-5 mm thick limit (m): 270.54 [ psi : 0.54 , Bar : 0.0375 ]
- 14. Glass break 3-5 mm thick limit (m): 1268.64 [ psi : 0.23 , Bar : 0.0159 ]
- 15. Loud noise 75-85 (dB) decibels (m): 1271.69

Computed distance at user entered psi/Bar

16. 5 psi given psi : 5.00 Bar : 0.3447 at distance : 26.97 (m)

## Validation scenario 3: Release of toxic chlorine

For ValidationCl2 HAMS-GPS: Dispersion Module

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Town)] Date: Friday, December 30, 2022

Data Entered

Reference No.: ChlorineValidation Name of Chemical: Chlorine

Scenario: 5. CLG Liquid Pipe leak One Min. Rapid Vaporization of Cryogenic Liquid Pool (SMOD-37 Pool dispersion DF)

Height of release (m): 1

Percent Humidity (%): 10.00 Height of simulation (m): 1

Atmospheric stability class: F

Wind velocity: 2.00 m/s at height 1.00 m

Terrain: Level

Rate of Release (g/Sec): 690

#### Results

Max Isopleth conc (ppm): 950000.00 Max. Isopleth Conc. Distance from source/release (m): 2.00

MGC (ppm): 10227.53 MGC Distance (m): 17971.54

Time for stabilization concentration zones of dispersion (Secs) 2.50 Flammable mass for VCE (lbm): N.A.

\*MGC: Maximum Ground Concentration in ppm

		Concentration (ppm):	Begin point (m)	End point (m)	Time (Sec)	Isopleth length (m)	Isopleth (Y-Axis) [m]	Distance of Max. ISOP from source [m]	Isopleth angle (deg.)	Isopleth Area (Ha)
Conc. 0	•	100	2.00	893.46	446.94	891.46	49.14	501.00	2.81	3.441
Conc. 1	•	50	2.00	1402.12	701.40	1400.12	72.30	798.00	2.59	7.950
TEEL3/IDLH:	•	20	2.00	2597.41	299.33	2595.41	123.47	1476.00	2.39	25.168
TEEL2:	•	5.8	2.00	6245.91	3124.46	6243.91	263.70	3544.00	2.13	129.317
TEEL1:	•	1.45	2.00	17972.54	8990.59	17970.54	655.59	10183.00	1.84	925.301
TEELO:	•	1.45	2.00	17972.54	8990.59	17970.54	655.59	10183.00	1.84	925.301

NOTE: 1. According to latest Emergency Planning, one has to use TEEL (Temporary Emergency Exposure Limits-15 min exposures) and ERPG (Emergency Response Planning Guidelines-1-hr. exposure) Limits are to be used. TEEL0 is Safe level, TEEL1 s mild action, TEEL2 is no irreversible effect and TEEL3 is life threatening and irreversible health effect. Incase Maximum Isopleth/at height of release Concentration is less than the lethal concentration then Conc1. Conc2, Conc3, and so on are assumed ppm values are entered which may be lower than lethal concentration.