



Consequence assessment considerations for toxic natural gas dispersion modeling[☆]

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ARTICLE INFO

Keywords:

Consequence modeling

Facility siting

Toxicity

Hydrogen sulfide

Impact zone

Parameter sensitivity

Natural gas composition

ABSTRACT

The numerical simulation of gas dispersion and estimation of consequence impact is of importance in Oil and Gas industry's process safety management. For natural gas fields with toxic components like Hydrogen sulfide, the toxicity impact zone drives business decisions related to equipment design, facility siting, layout, land use planning, and emergency response measures. Proprietary tools or empirical models which are calibrated using experiment database are often used for carrying out consequence modeling.

The selection of a software tool and a suitable dispersion model, based on the cloud behavior, at the source of dispersion is critical for the impact zone estimation. It is observed that, the fluid phase and the cloud density are key for determining the appropriate dispersion model. Incorrect parameter selection could lead to an inaccurate consequence impact zone estimation. This in turn could result in disproportionate process risk management efforts especially for toxic impacts from exposure to a very low concentration.

This paper discusses the results from consequence modeling studies done for a selected set of toxic natural gas release events related to onshore pipeline transfer using approved software. The study analyses the modeling inputs, parameters and determines the key release source terms and atmospheric parameters that impacts the estimation of impact zones. The study determined that the natural gas dispersion behaviour is dependent on the natural gas molar mass and the composition of Hydrogen sulfide. The study provides the guidance on overcoming uncertainty in dispersion modeling through sensitivity assessments and lists key parameters to be subjected for toxic natural gas dispersion modeling sensitivity analysis.

1. Introduction and motivation

Understanding of the process related risks is key attribute in process safety management of natural gas exploration and transportation. Several major toxic natural gas release incidents (see Table 1) have happened in the recent past resulting in human fatality, environmental damage and asset loss (BSEE; Jianwen et al., 2011; Stephens, 2000). Predictive risk assessments are carried out to determine the extent of hazardous level distances (impact zone) and how frequently the event occurs (Nair and Wen, 2019b).

Estimation of the potential impact zone from different accident scenarios through scenario-based consequence modeling forms integral part of process risk assessment (US DoT 2018). An important contribution to the calculation of the impact zone comes from the modeling of atmospheric dispersion following the accidental release of toxic fluids.

Impact zone estimation by consequence modeling is typically carried out using proprietary tools or empirical models (Hanna et al., 1982; Nair and Wen, 2019b). The commercially available models and tools have a range of applicability and are validated using experiments (Hanna et al., 1982; Pandya et al., 2012). Variation in the model inputs impact results and the model parameters have different influences on the results (US DoT, 2018). As per Nilsen et al., the computer tools can give substantially different results with respect to dispersion distances for the same accident scenario. The variations seem to be larger when the stagnant conditions are liquid or 2-phase (Nilsen et al., 2014).

In natural gas exploration and production industry, the risk management efforts including release event prevention and consequence mitigation are prioritized using the process risk assessment outputs which is based on the scenario-based consequence modeling and its likelihood. Facility siting and layout is a cost effective and powerful

[☆] (2020 Mary Kay O'Connor Process Safety Symposium October 20-21, 2020 | College Station, Texas).

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<https://doi.org/10.1016/j.jlp.2022.104792>

Received 25 October 2021; Received in revised form 26 January 2022; Accepted 2 May 2022

Available online 26 May 2022

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Table 1
Toxic natural gas Incidents.

Incident	Consequence and description
1950, Poza Rica, Mexico low altitude temperature inversion	Twenty-two persons died and 320 were hospitalized as a result of exposure to hydrogen sulfide for 20-min period.
1974–1991, Sour gas gathering line releases, USA (EPA records)	11 incidents, Multiple fatalities, Unspecified number of wildlife died
1992, Gezi, The Zhao 48# well; H ₂ S gas well blowout	6 fatalities and 24 poisoning; under pit operation corporation, Petroleum administration, Bureau of North China
2003, Kaixian blowout (Chongqing “12.23” incident), high sulphur gas	240+ fatalities, 2000+ hospitalization, 65000 evacuated; direct economic loss of \$900 million
2006, Sichuan (The Luo 2# well)	About 10000 people evacuated
2010–2014, Southeast Saskatchewan, Canada	43 sour gas leaking facilities (with average H ₂ S concentrations at 30,000 ppm)
2013, Kashghan field, Kazakhstan	200 km of leaking pipeline, \$3.6 billion to replace

design step in process risk management (Nair and Salter, 2019a). The potential impact zone (hazardous distances) from facilities, pipelines and units forms key information in site selection and layout optimization in multi-million projects. Incorrect selection of the consequence modeling approach, the software and any uncertainty in the input could lead to an inaccurate impact zone estimation which could result in disproportionate risk management efforts.

Note: This paper forms second part of the research study publications by the primary author under the guidance of third author. The first part of the research established that the depending on the gaseous mixture properties, and ambient conditions, the sour natural gas cloud from a release could be (i) dense (gravity slump), (ii) buoyant (rises over time), or (iii) neutrally buoyant (neither rises nor drops but disperses over time). The dispersion is seriously affected by the terrain, the loss of containment (leakage) conditions and surrounding conditions for e.g. wind speed. The second part of the research, reported in this paper determines the compositions of natural gas with shifts in buoyancy behaviours and identifies the parameters to be subjected to further detailed analysis. The first part used freely available software and the second part used commercially available software commonly used in Oil & Gas Industry. The third part of the research uses higher fidelity model (OpenFOAM, open-source Computational Fluid Dynamics software) to further assess the toxic natural gas dispersion behaviour in order to provide guidance on overcoming uncertainty in dispersion modeling (including software, solver, input and parameter selection).

2. Methodology and tools

Impact zones from potential outcomes like explosion overpressure, hazardous levels of toxic concentration, flammable cloud extent or thermal radiation from fires are estimated by (i) experiments/field trials, (ii) using index, spacing tables, (iii) predictive (consequence) modeling (IOGP, 2010). This study follows the scenario-based model approach for gas transmission integrity management risk assessment as per ASME B31.8S-2004 (US DoT, 2018) to determine the key parameters that

should be subjected to sensitivity analysis. The analysis focuses on the significance of toxic natural gas composition, release source terms and environmental parameters that could impact the dispersion and the estimation of impact zones. The key stages of consequence modeling are given in Fig. 1.

2.1. Hazard, scenario and input

Natural gas is a clean and naturally occurring hydrocarbon gas mixture which is an efficient source of energy. Natural gas in the event of unplanned release followed by ignition can result in flash fire, jet fire or explosion leading to thermal radiation or overpressure impact to personnel, environment or asset. Natural gas consists primarily of methane (CH₄) and rest of the composition depends on the reservoir (gas field) location. One-fifth to one-third of all natural gas resources in the world could fall under the sour gas classification (Kelley et al., 2011). Natural gas is usually considered ‘sour’ if there are more than 5.7 mg of H₂S per cubic meter of natural gas, which is approximately equivalent to 4 ppm by volume under standard temperature and pressure (Speight, 2007). H₂S is highly toxic (fatal effects at low concentration), extremely flammable and corrosive. The molecular mass of CH₄ is 16 lb/lbmol (lighter than air) and that of H₂S is 34.1 lb/lbmol, slightly heavier than air (29 lb/lbmol) at standard conditions. Pipeline accidents accounted for 70% of the accidents involving natural gas and the most frequent causes were mechanical failure of the pipelines or due to significant changes to the surrounding environment (Bariha et al., 2016). 90% of sour natural gas releases could result in toxic cloud dispersion with potential impacts (Muhlbauer, 2004).

Accidental releases of toxic natural gas from transfer pipeline (pipeline from wells to gathering stations and processing facilities/treatment plant) and atmospheric dispersion was considered for this evaluation. The treatment plants, a common one for a large production field area, has a network of pipeline which sometimes has to be routed through populated areas (Speight, 2007). A ground level release from

Table 2
Input, parameters and sensitivity values.

Input/Parameter	Base value	Sensitivity values
Release source term		
Hole size	2 in	1 in, 3 in
Temperature	Medium (77 °F)	Low (20 °F), High (120 °F)
Pressure	Medium (115 psia)	Low (50 psia), High (500 psia)
Orientation	Horizontal (1° from grade)	Upwards (45° from horizontal)
Environmental parameter		
Atmospheric stability	Stable (F)	Neutral (C, D)
Wind speed	Low (3.4 mph)	Med (13 mph), High (20 mph)
Humidity	Medium 50%	Low (20%), High (80%)
Terrain (surface roughness)	Med – Level country/Cut grass (0.2 in)	Low – Mud flats, Snow (0.0004 in) High – Wooded/urban area (3.9 in)

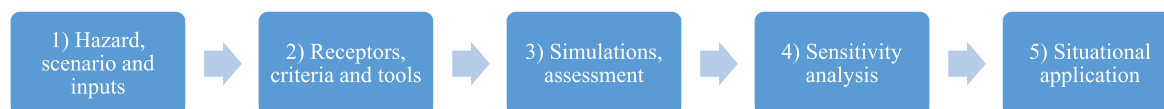


Fig. 1. Methodology - Consequence modeling and sensitivity analysis.

Table 3

Toxic natural gas composition (mol %).

Natural gas composition	S1	S2	S3	S4	S5	S6	S7	S8
Water	1.7%	3.0%	1.0%	0.7%	0.3%	0.0%	0.0%	1.0%
Nitrogen	0.1%	0.4%	0.5%	0.9%	1.2%	1.0%	1.1%	0.3%
H ₂ S	2.6%	7.2%	9.6%	13.8%	14.1%	15.7%	17.0%	28.0%
CO ₂	5.4%	8.1%	11.2%	2.2%	3.3%	3.1%	8.3%	3.2%
C1	14.1%	49.6%	50.3%	78.1%	63.9%	57.4%	18.3%	35.0%
C2	28.0%	10.1%	9.5%	0.7%	10.1%	10.5%	24.0%	14.7%
C3	32.3%	9.7%	8.3%	0.9%	4.1%	5.8%	19.6%	10.7%
i-C4	3.3%	2.2%	2.0%	0.3%	0.6%	1.3%	0.0%	1.6%
n-C4	9.8%	4.4%	3.4%	0.7%	1.2%	3.0%	7.9%	3.1%
C5s	2.7%	3.4%	2.7%	0.7%	0.6%	1.8%	2.4%	1.6%
C6+	0.3%	2.0%	1.6%	0.9%	0.4%	0.5%	1.4%	0.8%
Molar mass (lb/lbmol)	38.3	30.2	29.9	21.7	24.2	26.7	36.8	31.7
Gas density @ 700 psi	6.03	3.42	3.82	2.54	3.22	3.82	5.61	4.18

pipeline (6-inch diameter) transferring toxic natural gas and downwind dispersion of the cloud was considered as the base case event scenario. Input and parameters for consequence modeling are given in [Table 2](#).

Three representative hole sizes (small, medium and large) was considered for the study and the hole sizes were selected to represent the releases resulting from typical loss of fixed equipment (pipeline) integrity (e.g. corrosion, erosion) or from operational upsets (e.g. blocked outlet).

Toxic natural gas from eight reservoirs across different geographic regions were analysed. The natural gases considered (represented as S1 to S8) include H₂S composition ranging from 2 to 28 mol% are shown in [Table 3](#). The gas densities at 700 psia are shown at the gathering system supply pressure for a typical reservoir.

2.2. Criteria and software tools

Tools: The study utilized commercially available and validated tools:

- (i) Aspen HYSYS for phase equilibrium estimations
- (ii) Canary by Quest for consequence (release and dispersion) modelling.

Aspen's HYSYS is an Industry's leading process simulation software and Canary by Quest is an United States Environmental Protection Agency approved integrated model for consequence assessment.

Criteria: Toxic and flammable cloud dispersion to concentrations of personnel impact are analysed through modeling. The hazardous concentration levels (to determine the distance to the dispersion end points) used for this study is given in [Table 4](#).

2.3. Simulations and results

Phase-equilibrium estimation (Aspen HYSYS): For this analysis, the

HYSYS process simulator was used to perform flash and property calculations to better understand fluid phase behaviour under process and release conditions. The Peng-Robinson (PR) equation of state (EOS) was used because it provides better phase and equilibrium estimations close to/at the critical point as well provide better liquid densities estimations for gas and condensate systems when compared to Soave-Relich-Kwong EOS and Non-Random Two-Liquid EOS ([Guerra 2006](#), [AspenTech, 2013](#)). Furthermore, AspenTech, the licensor for the HYSYS software, has made several enhancements to the original PR EOS model to extend its range of applicability (Temperature, Pressure, and binary interaction parameters) to improve predictions of non-ideal systems ([AspenTech, 2013](#)). Phase envelopes for each sample was generated using the phase envelope tool in HYSYS and used to verify canary input phase equilibrium calculations.

Distance to downwind dispersion estimation: For this study, Canary by Quest ([Canary by Quest](#)), a regulator approved consequence assessment software, is used to determine the potential impact distance following hazardous fluid release. Canary has a range of validated auxiliary models including models which integrates multicomponent thermodynamics into the time-varying fluid release simulation ([Tauseef et al., 2017](#)). The base models in Canary are derived from DEGADIS and SLAB (available in public domain) and validated ([US EPA, 2017](#)).

The study focuses on a selected set of scenarios to represent the release from a toxic natural gas transfer pipeline to treatment plants in the onshore natural gas exploration and production. Consequence modeling (release and dispersion) from 2-inch hole in horizontal direction at ground level for stable wind condition and low wind speed was carried out and considered as the base case for this study. The flow through pipeline is fixed at 50 lb/s and release from a hole is assumed to be continuous (60 min) and disperses in an open field (no impingement). The number of components in the toxic natural gas compositions was optimized (given [Table 5](#)) for more accurate phase representation within the Canary multi-component model. Using the phase envelope generated from HYSYS, the input compositions were modified to ensure

Table 4

Hazardous levels for natural gas release evaluation.

Component	Accidental consequence	Level-3	Level-2	Level-1
Natural gas (see values in Table 5)	Flash fire (flammable vapor cloud distance)	Upper Flammability Limit (UFL) Methane (CH ₄) 16% Propane (C ₃ H ₈) 9.5%	Lower Flammability Limit (LFL) CH ₄ 4% C ₃ H ₈ 2%	50% LFL CH ₄ 2% C ₃ H ₈ 1%
Hydrogen sulfide (H ₂ S)	Toxic concentrations of exposure results in health effects or death	500 ppm potential for respiratory arrest, loss of consciousness	100 ppm Immediately dangerous to life and health (IDLH), coughing, dizziness	75 ppm Acute Exposure Guideline Level #3; loss of sense of smell in minutes

Table 5

Multi-component compositions for release and dispersion modelling (mol %).

Natural gas composition	S1	S2	S3	S4	S5	S6	S7	S8
H ₂ S	2.6%	8.1%	10.4%	14.3%	14.6%	16.5%	17.8%	29.6%
CO ₂	5.5%	9.1%	12.1%	2.2%	3.4%	3.3%	8.8%	3.4%
CH ₄	14.3%	55.7%	54.5%	81.0%	66.1%	60.1%	19.2%	37.0%
C ₂ H ₆	28.5%	11.3%	10.3%	0.8%	10.4%	11.0%	25.3%	15.5%
C ₃ H ₈	32.8%	10.9%	9.0%	0.9%	4.3%	6.1%	20.6%	11.3%
C ₄ H ₁₀	13.3%	4.9%	3.7%	0.8%	1.3%	3.1%	8.3%	3.3%
Molar mass (lb/lbmol)	38.7	27.7	26.8	20.0	22.8	24.5	34.5	29.1
UFL	11.3%	15%	16%	16.6%	16.1%	15.8%	14.3%	16.6%
LFL	2.6%	4.0%	4.2%	4.8%	4.3%	4.1%	3.2%	3.7%

similar sample molar mass and H₂S composition which is acceptable for this comparative study. The analysis helped to understand the influence of user-adjustable parameters on model outputs.

For the risk assessment using integrated software, the width of the cloud and the averaging time plays a significant role (US EPA, 2017). In this study, the results of dispersion were recorded for the maximum concentration along downwind central line concentration for an averaging time of 60 s.

2.4. Uncertainty and sensitivity analysis

In order to develop confidence in understanding a model, evaluate how variations in a model's outputs can be apportioned to variations in the inputs, which often referenced as sensitivity analysis (IOGP, 2010, Pandya et al., 2012; US EPA, 2017). Sensitivity analysis approach by varying one input parameter at a time which holds other parameters at central values. The sensitivity outcomes are dependent on these central values. Each of the eight toxic gas compositions, were subjected to the sensitivity to the range of values for input and parameters. The results are presented using histograms or quantitative measures to compare the sensitivity of the uncertain input and parameter.

3. Results and discussion

This section reports the results of the simulations and discuss the sensitivity to the input and parameters. The aim is to identify the most

important parameters from amongst a large number that affect model outputs. This will help in optimizing the time and resource usage for consequence modelling in risk assessment. The analysis is carried out on two sets:

- Material and release conditions (Source term): fluid composition, hole size, temperature, pressure, release orientation
- Environmental conditions: atmospheric stability, wind speed, humidity, terrain

3.1. Sensitivity: fluid composition

Over the years, certain heuristics have been used as source term input parameters for modeling multiphase releases and ensuing dispersion. Examples of these heuristics include choosing a pure component of the same molecular weight in place of the mixture, distilling mixture composition to a handful of components, choosing to model natural gas as a pure methane, etc. Although convenient, these modeling assumptions can result in hazard estimations that diverge from reality with the biggest problem being the inability to accurately account for thermodynamic effects like phase splits and composition changes during release conditions (Johnson and Marx, 2003).

Pressure-Temperature (P-T) projection (estimated using HYSYS) of the phase diagram of a multicomponent system is compared against pure material and a simplified composition. Fig. 2 illustrates the P-T

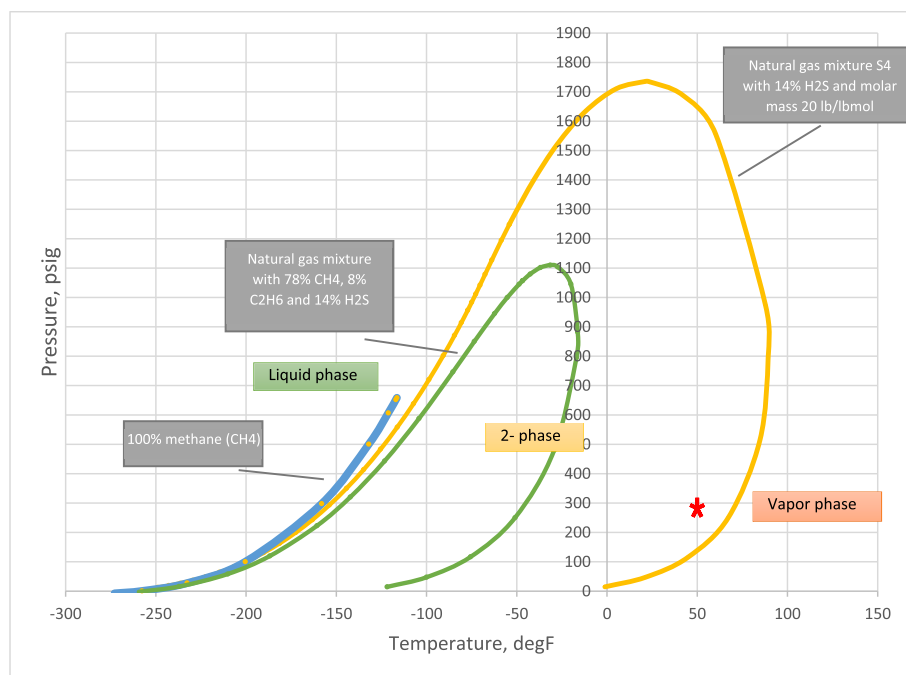


Fig. 2. Phase equilibrium curves for methane (blue), Methane-ethane-Hydrogen sulfide (green), and S4 Natural gas (yellow). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

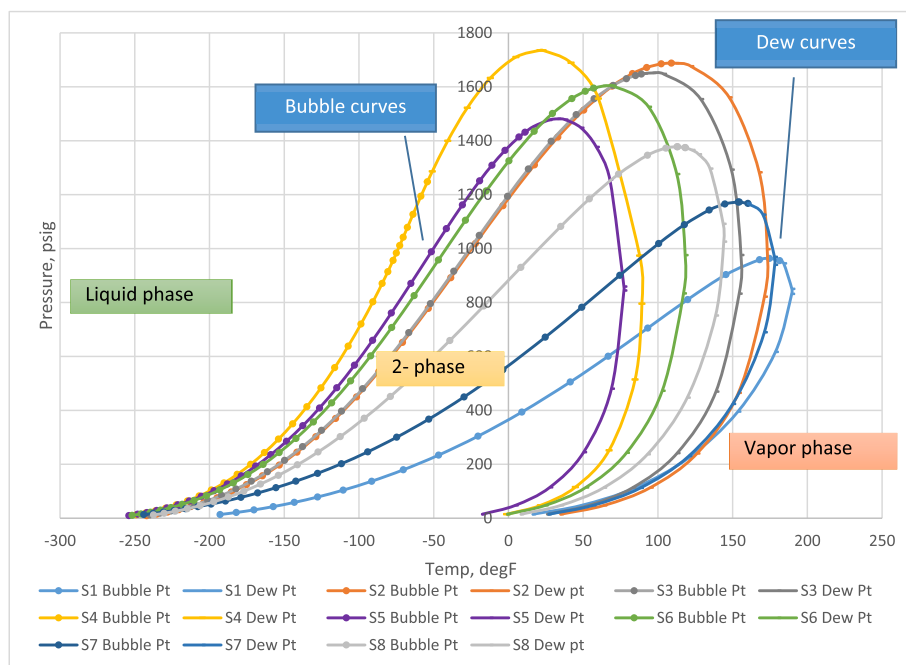


Fig. 3. Phase equilibrium curve – toxic natural gas compositions.

projection of natural gas. A typical set of natural gas pipeline transfer operating conditions are considered, 50 degF and 300 psia (red mark in the figure), for the comparison.

Going by the popular heuristic of modeling natural gas as 100% methane (blue line), it was observed that at the pipeline operating conditions, the release is purely vapor with buoyant properties. Similarly, if the natural gas mixture with three components (78% CH₄, 8% C₂H₆ and 14% H₂S) represented by the green line, at the pipeline vapor is mostly vapor too. However, a detailed composition of the mixture (S4, Table 5) reveals the release contains vapor, aerosol, and liquid phases which were missed in the other two compositions.

For this study, the compositions analyzed (Table 5) include toxic gases with molar mass lower, similar and higher than that of air (28.9 lb/lbmol) in order to factor in the potential buoyancy effects in the toxic cloud dispersion. A comparison of the molar mass and H₂S composition also shows that the molar mass of the toxic natural gas is not directly proportional to H₂S mol% nor to any one pure hydrocarbon component. The phase envelope of eight compositions toxic natural gas given in Fig. 3 illustrates that the phase of a multicomponent toxic natural gas could vary (liquid, 2-phase or vapor) with a change in the composition, temperature and pressure.

Density of fluid and related buoyancy (positive, neutral, negative) plays a major role in selecting the dispersion modelling approach (passive, dense etc) for estimating downwind distances (Nair and Wen, 2019b). Released fluid density is driven by fluid's molar mass molar mass, release pressure and temperature. The Bubble curve and the Dew

curves shift towards to right with an increase in molar mass (S1, S7, S8). This is due to the higher molar mass from higher composition of C4+ hydrocarbons and hydrogen sulfide contribution. The phase of the released material is critical since it determines the release and dispersion model used (e.g. heavy gas vs gaussian); an inappropriate selection can lead to erroneous results. For example, the fluid phase of S5 (MW 24.2) and S6 (MW 26.7) with similar molecular mass could yield different results for a given pipeline operating pressure and temperature; for example, at 800 psig and 100 °F, S5 will be vapor, whereas S6 will be 2-Phase. Discussion on the sensitivity to the changes in temperature and operating pressure is included in section 3.3.

Dispersion modeling was carried out with base case inputs for all eight toxic natural gas compositions (Table 5) using Canary by Quest. The estimated downwind distances (impact zones) to toxicity and flammability criteria (Table 4) is given in Table 6.

The downwind distances for LFL ranges from 27 ft (S4, S5) to 60 ft (S1) and H₂S 100 ppm cloud ranges from 820 ft (S2) to 1775 ft (S8). The following observations inferred from the results:

- Distance to H₂S toxic hazard level is significantly larger than flammability hazard levels. For example, results of toxic gas composition S2, toxicity downwind distance to 500 ppm = 261 ft and 100 ppm = 820 ft whereas the flammable cloud downwind distance UFL = 8 ft and LFL = 30 ft). Hence, for natural gas with toxicity, it can be inferred that the hazard level distances are driven by toxicity impact.

Table 6

Downwind dispersion distances to base case toxic and flammable criteria.

Natural gas	Molar mass	H ₂ S mol %	Distance downwind (ft) to H ₂ S concentration			Distance downwind (ft) to flammable concentration		
			500 ppm	100 ppm	75 ppm	UFL	LFL	0.5LFL
S1	38.7	2.6%	370	1110	1338	20	60	110
S2	27.7	8.1%	261	820	985	10	32	55
S3	26.8	10.4%	320	965	1150	8	30	52
S4	20.0	14.3%	408	1185	1410	8	27	49
S5	22.8	14.6%	411	1190	1415	8	27	49
S6	24.5	16.5%	450	1285	1520	8	31	55
S7	34.5	17.8%	480	1327	1565	10	40	69
S8	29.1	29.6%	668	1775	2085	8	34	60

- ii. Downwind distance of toxic dispersion is maximum for those release with higher compositions of H₂S (S7, S8) and with higher molar mass (S8, S7, S1). Downwind distance of flammable cloud dispersion is higher for composition with higher molar mass (S1, S7).

3.2. Impact of water vapor in natural gas

Well fluids may become saturated in the presence of produced water during production and transmission. As part of the analysis in this paper, the impact of water saturation on natural gas (with H₂S) dispersion in the event of a release was studied. Using the water saturate tool in Aspen HYSYS, S6 natural gas sample was saturated at 115 psig and 77 degF to estimate the new composition given in Table 7.

Consequence modeling was performed using Canary to assess the impact of water saturation on downwind dispersion to H₂S hazard level dispersion distance (see Fig. 4).

The difference in the estimated downwind distances (about 1%) for the dry and saturated natural gas is not significant for the process risk management purposes. The results suggest that water saturation of natural gas is not a significant parameter in downwind dispersion to H₂S hazard levels.

Table 7
Wet (saturated) and Dry base – natural gas (S6) compositions (mol%).

Component	Dry basis	Wet basis
H ₂ O	0.00%	0.15%
Nitrogen	1.00%	1.00%
H ₂ S	15.68%	15.66%
CO ₂	3.10%	3.09%
Methane	57.34%	57.25%
Ethane	10.49%	10.47%
Propane	5.79%	5.79%
i-Butane	1.30%	1.30%
n-Butane	3.00%	2.99%
n-Pentane	1.80%	1.80%
n-Hexane	0.50%	0.50%

3.3. Release source terms and sensitivity

In the literature review and simulations carried out using ALOHA by Nair & Wen, it is evident that the existing so called simple models and algorithms cannot adequately consider H₂S specific properties for the toxic natural gas dispersion (Nair and Wen, 2019b). ALOHA is a program developed by the US EPA Chemical Emergency Preparedness and Prevention Office and the National Oceanic and Atmospheric Administration Office of Response and Restoration and is part of the agency's Computer-Aided Management of Emergency Operations (CAMEO) suite.

3.3.1. Source term sensitivity to release rate

The necessity of natural gas composition accuracy to the Canary model input values release hole size, temperature and pressure is evaluated in this section. Base case scenario is a release from 2-inch hole in horizontal direction at ground level. The flow through pipeline is fixed at 50 lb/s with operating temperature 77 °F and pressure 115 psia. Simulations were run for a higher and lower value and the release rates were estimated. The sensitivity values used as per Table 2 and the results are given in Table 8.

The following observations were inferred from the results:

Release rate comparison for release hole sizes (1, 2 and 3 inch):

- Release rates grow significantly with increase in hole size irrespective of the composition. For S1 composition, the release rates varied from 2.9 lb/s to 21.5 lb/s.
- Release rates were higher for compositions with larger molar masses (S1, S7) and the difference is significant for larger hole sizes.
- Similar release rates (e.g. 11.5–12.7 lb/s, 3-inch hole) for compositions with molar mass less than 27 lb/lbmol (S2, S3, S4, S5, S6) for all hole sizes. However, significantly higher release rate (21.5 lb/s) for S1 with molar mass 39 lb/lbmol.

Release rate comparison for operating pressures (50 psig, 117 psig and 500 psig):

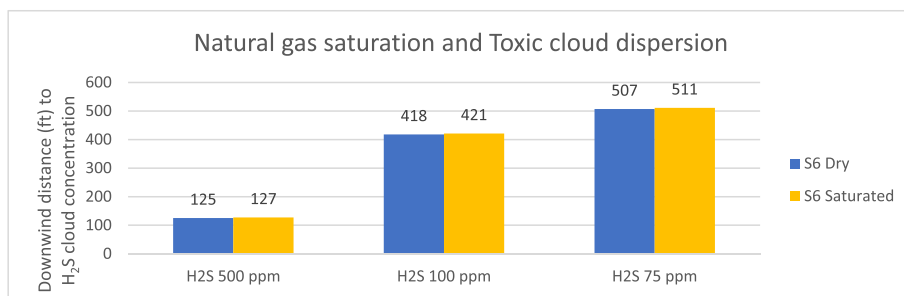


Fig. 4. Sensitivity – natural gas saturation: Downwind distance to H₂S concentration.

Table 8
Comparison of release rate (lb/s) for hole size, pressure and temperature.

Natural gas composition	Molar mass	H ₂ S mol %	Base case	Release hole		Pressure		Temperature	
			2 inch, 77 °F, 115 psia	High (3 inch)	Low (1 inch)	High (500 psia)	Low (50 psia)	High (120 °F)	Low (20 °F)
S1	38.7	2.6%	11.8	21.5	2.95	50 ¹	3	11.8	16.2
S2	27.7	8.1%	5.7	12.7	1.42	28	2.5	5.7	6.25
S3	26.8	10.4%	5.9	12.7	1.43	28	2.5	5.9	6.25
S4	20.0	14.3%	5.1	11.5	1.27	23	2.2	5.1	5.45
S5	22.8	14.6%	5.4	12.2	1.35	25	2.3	5.4	5.8
S6	24.5	16.5%	5.6	12.6	1.4	26.5	2.4	5.6	6.05
S7	34.5	17.8%	6.7	15	1.66	50 ¹	2.8	6.7	12.3
S8	29.1	29.6%	6.1	13.7	1.54	50	2.6	6.1	6.6

Note: ¹ For S1 and S2 composition and High pressure, the release is two-phase.

- i. For low pressure, the release rates were between 2 and 3 lb/s for all compositions.
- ii. For medium pressure, the release rates ranged from 4.5 to 5.5 lb/s for all compositions (S2 to S8) with molar mass less than 29 lb/lbmol, but higher (11.8 lb/s) for S1 with the highest molar mass.
- iii. For high pressure, the compositions (S1, S7, S8) with higher molar mass (>29 lb/lbmol) have significant higher release rates (>38 lb/s) compared to the compositions (S2, S3, S4, S5, S6) with lower molar mass (<29 lb/lbmol).

Release rate comparison for operating temperature (20 °F, 77 °F, 115 °F):

- i. For medium and high temperature conditions, the release rates are similar irrespective of the compositions.
- ii. Similar release rates (~5 lb/s) were estimated for compositions with molar mass 29 lb/lbmol and less for the range of temperatures evaluated.
- iii. Significantly higher release rates were estimated for compositions with molar mass greater than 30 lb/lbmol under low temperature conditions.

3.3.2. Source term sensitivity to dispersion

The downwind dispersion distance sensitivity to the source terms (hole size, operating temperature and pressure) are discussed in this section.

Downwind dispersion comparison for release hole sizes (1, 2 and 3 inch) see Fig. 5:

- i. Downwind dispersion distance to 500 ppm H₂S concentration from small (1-inch) hole releases was noted as proportional to the H₂S composition. However, for larger hole sizes the increase in downwind distance was not proportional to the change in hole size.
- ii. Longest downwind dispersion reported (3inch releases), for 500 ppm H₂S concentration was for S8 composition (28% H₂S, molar mass = 29 lb/lbmol), while 100 ppm was for S7 (18% H₂S, molar mass = 34

lb/lbmol). Downwind dispersion following release from larger hole sizes are influenced by H₂S concentration and molar mass.

Downwind dispersion comparison for operating pressures:

Dispersion for eight natural gas compositions at three pressure conditions (low = 50 psia, medium = 117 psia, high = 500 psia) and the downwind distances to 500 ppm and 100 ppm H₂S was estimated (see Fig. 6).

During expansion from elevated pressure, released toxic gas could be colder and heavier than air close to the release source with the potential to accumulate in low-lying areas (Nair and Wen, 2019b). From the simulations, it is established that the cloud dispersion behaviour changes to dense gas for natural gas with H₂S compositions higher than 18 mol%. For high H₂S compositions (S7, S8), the dispersion distances were significantly longer for high pressure releases (500 ppm exceeds 2750 ft compared to less than 1000 ft for natural gas with less than 18% H₂S).

Downwind dispersion comparison for operating temperatures:

Dispersion for eight natural gas compositions at three temperatures (low = 20 °F, medium = 77 °F, high = 120 °F) and the downwind distances to 500 ppm and 100 ppm H₂S was estimated (see Fig. 7).

- i. For all three temperature conditions, downwind dispersion distances similar for all compositions with molar mass less than 30lb/lbmol.
- ii. Downwind dispersion distances for composition with greater than 30lb/lbmol similar for medium and high temperature, whereas significantly higher for low temperature releases.

Downwind dispersion comparison for Release orientation:

Release and dispersion from two release orientations, horizontal and upwards (at 45deg from horizontal) for the eight natural gas compositions and from 2-inch hole at 77 °F and 115psia were compared (see Fig. 8).

- i. Downwind dispersion distances are higher for horizontal orientation compared to upwards orientation for all compositions.

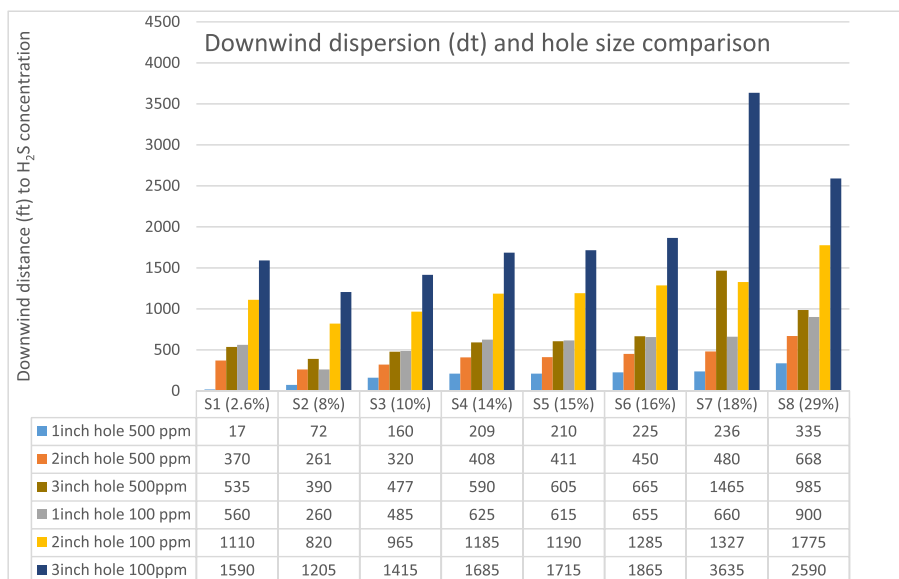


Fig. 5. Sensitivity of downwind distance (H₂S concentration) to Release hole size.

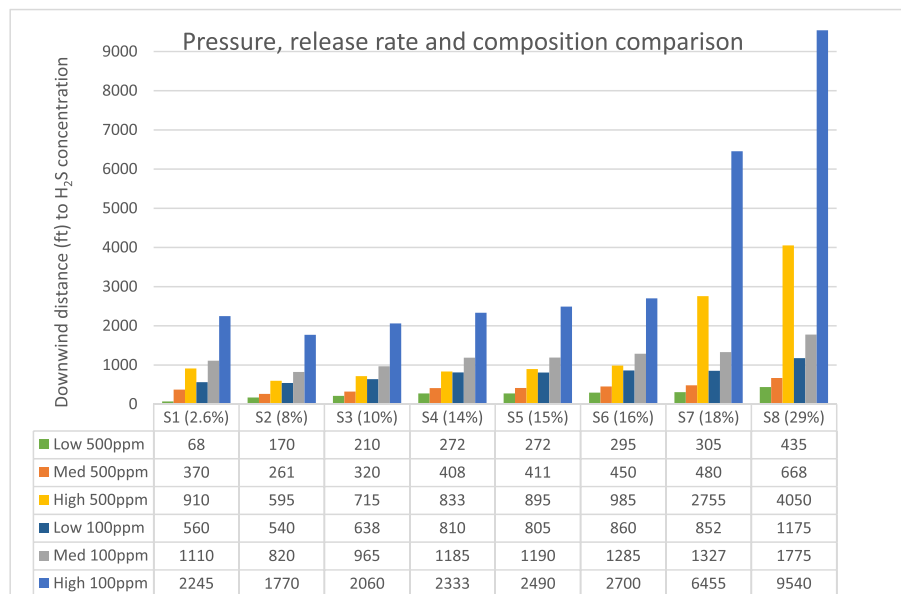


Fig. 6. Sensitivity of downwind distance (H_2S concentration) to Operating pressure.

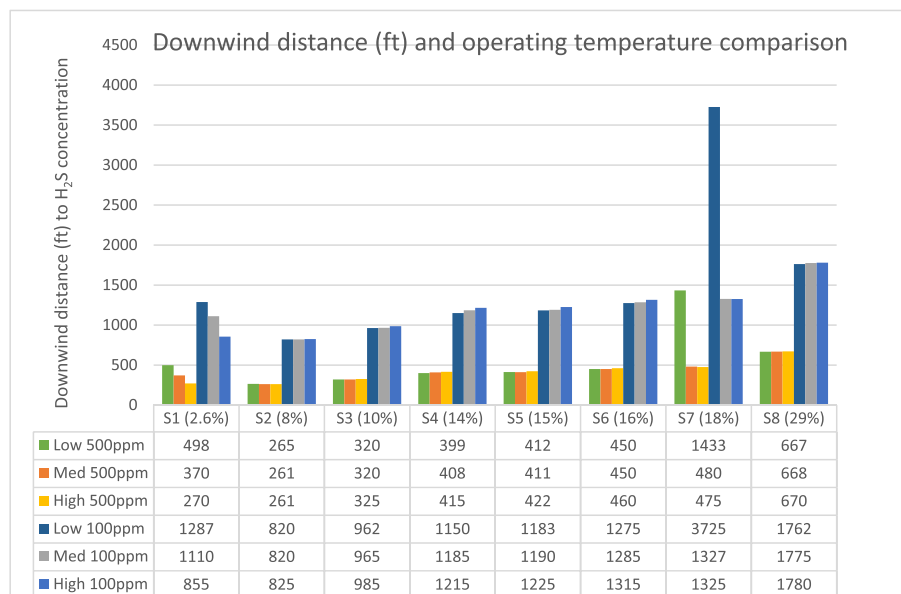


Fig. 7. Sensitivity of downwind distance (H_2S concentration) to Operating temperature.

- ii. For both orientation, downwind dispersion distances for 500 ppm and 100 ppm were similar for compositions with H_2S concentrations 14%–18% (S4, S5, S6, S7), but significantly lower for compositions with low (<10%) H_2S concentrations (S1, S2) and significantly higher for compositions with high (>20%) H_2S concentrations (S8).
- iii. For dispersion from upwards releases, the downwind dispersion distance increases with the increase in H_2S concentration. For dispersion from horizontal release, S1 with 2.6% H_2S (highest molar mass and release rate) dispersion distances are higher than S2 (8% H_2S) and S3 (10% H_2S).

Appropriate orientation based on the failure mode and expected location (elevation) of the receptors of concern should be used for consequence modeling.

3.4. Environmental parameters and sensitivity

3.4.1. Sensitivity – atmospheric stability and wind speed

Dispersion for set of eight natural gas compositions and from 2-inch hole at 77 °F and 115 psia under three atmospheric stability conditions and wind speeds (3.4F: stable and low wind speed, 13D: Neutral and medium wind, 20C: slightly unstable and high wind) were compared. Following observations, were inferred from the results given in Fig. 9.

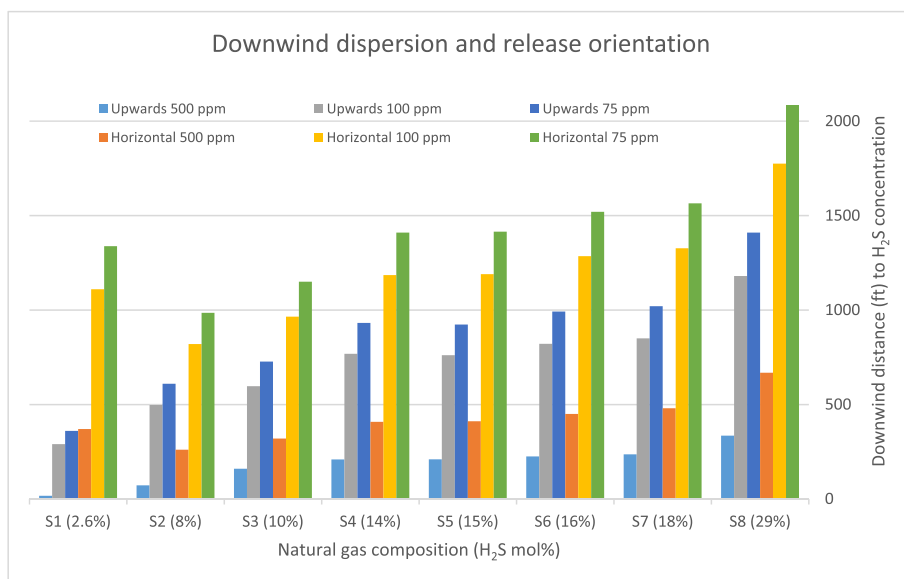


Fig. 8. Sensitivity of downwind distance (H_2S concentration) to Release orientation.

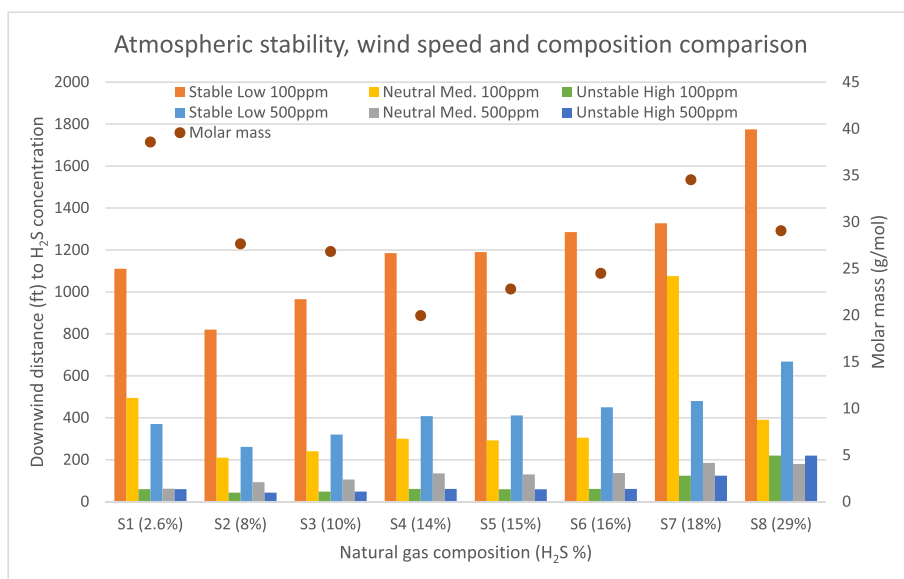


Fig. 9. Sensitivity of downwind distance (H_2S concentration) to Atmospheric stability and wind speed

Note: Canary tool couples (transition) from jet dispersion to heavy gas dispersion when the central line touches ground level. This modeling factor is reflected in results for S7 under 13D conditions and for all compositions under 20C conditions.

- The longest downwind dispersion irrespective of the composition was recorded for stable conditions and low wind speed.
- For dense gas (negatively buoyant) compositions (S1, S7) with higher molar mass (>29 lb/lbmol), the downwind dispersion for Neutral and Medium wind (13D) was significantly higher.
- For lightly unstable and high wind speed (20C) conditions, the downwind distances for 100 ppm was less than 200 ft for all compositions whereas for stable and low wind speed (3.4F) conditions, the distances exceeded 800 ft.
- For compositions with molar mass <29 lb/lbmol (positively buoyant), the downwind distance for 20C conditions are higher than 13D conditions. Under these conditions, the cloud is behaving more as heavy gas and closer to ground level, whereby higher concentration cloud travels further downwind.

For higher H_2S concentration (S8 composition), the downwind

distance to 100 ppm extends to 1775 ft at low wind and stable conditions (3.4F) compared to 390 ft and 220 ft for neutral stability and higher wind speeds. For a location with predominant neutral stability and medium wind speed (like 13.4D), if the risk management bases the impact zone distance worst-case stability and wind (1775 ft) which is about 5 times typical (390 ft), then the risk management (e.g. emergency planning) incur significantly higher cost and effort.

3.4.2. Sensitivity – terrain

Dispersion for different toxic gas compositions and from 2-inch hole at 77 °F and 115 psia over three different terrains (mud flat, level country or cut grass, urban area) were compared. The terrains were considered flat (without obstructions) and the turbulence from terrains were addressed by surface roughness parameter as given in Table 2. Following observations are inferred from the results given in Fig. 10.

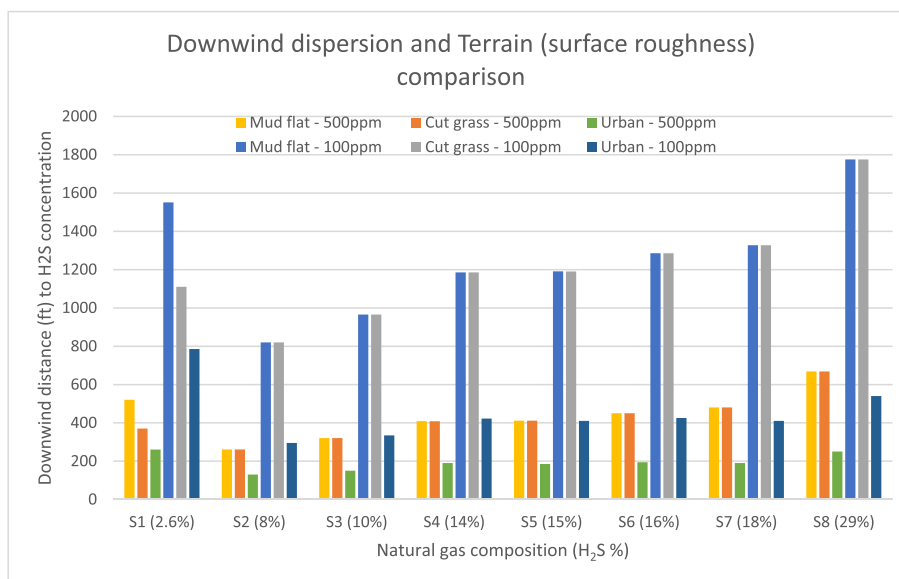


Fig. 10. Sensitivity of downwind distance (H₂S concentration) to Terrain.

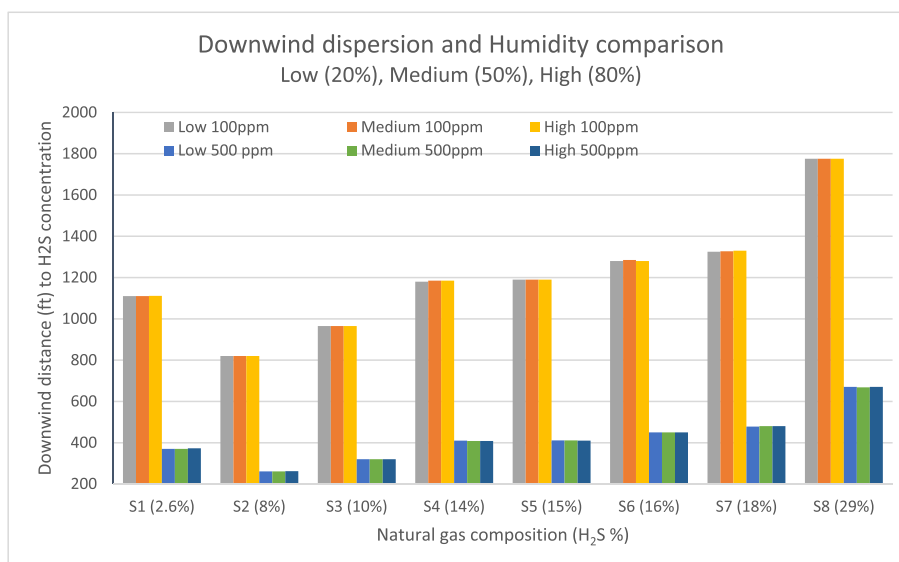


Fig. 11. Sensitivity of downwind distance (H₂S concentration) to Humidity.

- (i) With increase in surface roughness, the downwind dispersion decreases. Downwind dispersion distances for Urban area was significantly lower than (1/3rd) for all compositions except S1.
- (ii) Downwind dispersion distances for Mud flat and Cut grass is similar for all compositions except S1 with the highest molar mass. This implies that dispersion of toxic gas with less than 35 lb/lbmol molar mass is not sensitivity to surface roughness <0.2 inch.

3.4.3. Sensitivity – humidity

Dispersion for different toxic gas compositions and from 2-inch hole at 77 °F and 115 psia at three humidity conditions (low = 20%, medium = 50%, high = 80%) were compared. Results given in Fig. 11 implies that changes in humidity values has no significant impact on the downwind dispersion of toxic natural gas.

3.5. Application of the consequence modeling results in risk assessment

Significance of the consequence modeling results in the risk management efforts is analysed with the methodology, software and inputs were applied to a credible release event from pipeline routed through a populated area. The results from the parameter sensitivity analysis for natural gas composition S4 transposed to geographical location as pointed in Fig. 12. The potential impact to public (personnel) corresponding to each impact zone radius was estimated for comparing the levels of risk. A comparison with composition S7 and possible risk management considerations are also discussed. The downwind distances to 100 ppm H₂S cloud is summarized in Table 9.

Impact zones for selected few cases are illustrated in Fig. 12., the yellow pin corresponds to the release point and the colored circles represents the impact zone for different set of input and parameters are given in Table 7. The impact area for a release event will be a section of the circle with orientation dependent on the wind direction.

The representative set of cases with impact zones, corresponding

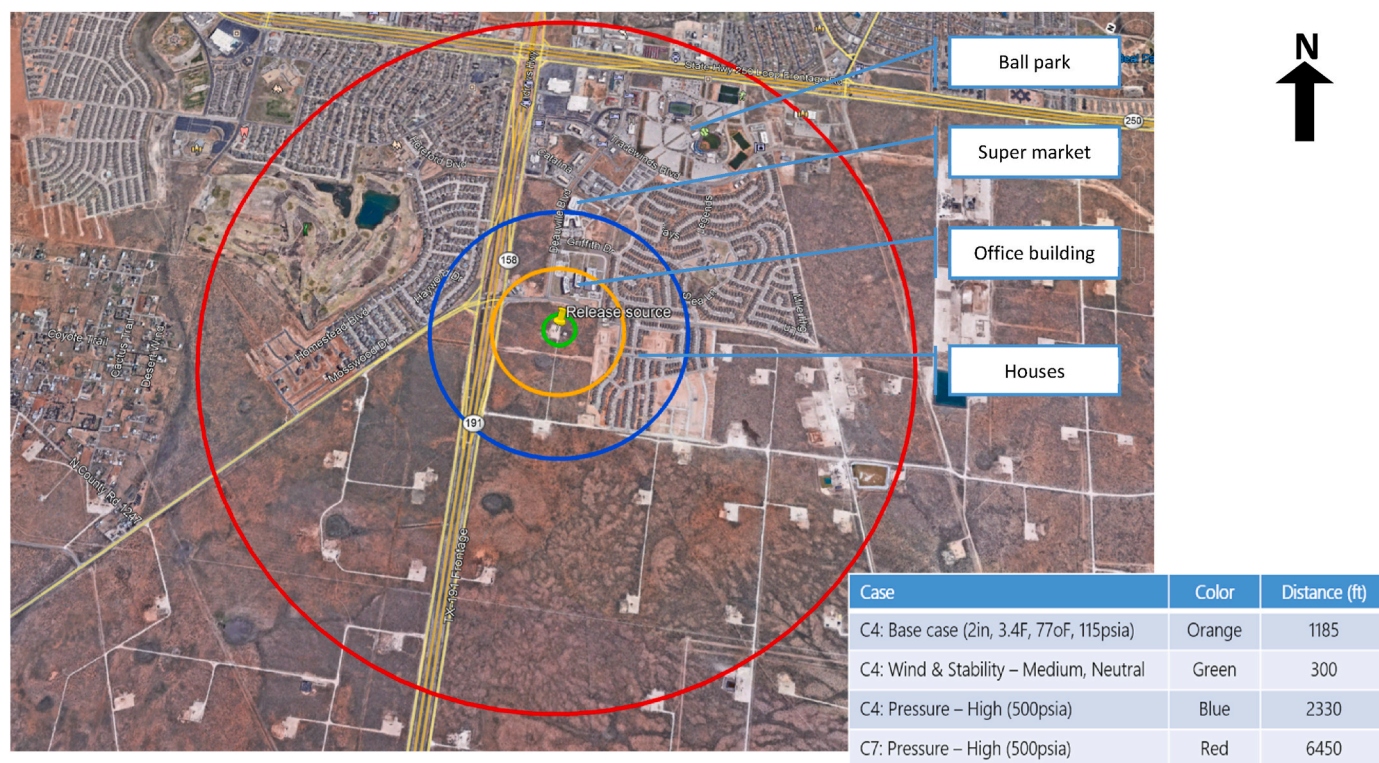


Fig. 12. Parameter sensitivity summary - H₂S downwind distances and potential impacts.

Table 9

Natural gas (S4) compositions (mol%) and downwind distance to 100 ppm H₂S.

Case sensitivity (distance in ft)	S4	S7
Molecular weight	20	35
Base case (2in, 3.4F, 77 °F, 115psia)	1185	1327
Sensitivity: Temperature – Low (20 °F)	1150	3725
Sensitivity: Pressure – High (500psia)	2330	6450
Sensitivity: Wind & Stability – Medium, Neutral	300	1075
Sensitivity: Surface roughness – High (0.1m)	420	410

Table 10

Natural gas impact zone – parameter sensitivity and risk management considerations.

Case sensitivity	Color	Consequence/concern	Risk management considerations
C4: Base case (2in, 3.4F, 77 °F, 115psia)	Orange	500+ (1 x Office, 30 houses)	Perform site specific assessment Risk reduction through buried lines, smaller diameter pipeline
C4: Wind & Stability – Medium, Neutral	Green	Environmental impact	Manageable risk, maintain exclusion zone
C4: Pressure – High (500psia)	Blue	2000+ (2 x office, 100+ houses)	Operational controls (e.g. at lower pressure)
C7: Pressure – High (500psia)	Red	25,000+ (Ball park, Supermarket, neighbourhoods)	Elevated risk, consider alternate route

potential consequence and risk management considerations are given in Table 10. The base case impact zone (Orange color and radius 1185 ft), the 100 ppm H₂S cloud (IDLH – concentration level) could reach an office building or residential area. This implies that in the event of a release under the given base case conditions and Southerly (towards North) wind, more than 500 personnel could be exposed to natural gas

cloud with 100 ppm or more for a period until the release is isolated and such an exposure could result in coughing and dizziness. Risk reduction measure considerations should be to reduce the impact zone radius including reducing the pipeline diameter or restricting the horizontal release orientation (e.g. laying pipeline underground). However, modeling using the site-specific representative wind speed and atmospheric stability (13D - medium and neutral) instead of worst-case conditions (3.4F – stable and low wind conditions), the impact zone estimated was much smaller (300 ft, Green color). The impact zone was limited to the facility surroundings (without personnel exposure) and whereby the risk management limits were limited to maintaining the exclusion zone (restricting personnel access/habitats). Similarly, for the impact zone and potential consequences for operating under higher pressure or for S7 composition is given in Table 10.

A worst-case consequence modelling estimate may not be the best for risk management, instead a ‘credible’ worst-case scenario needs to be determined and subjected to consequence modeling. The credibility of a set of modeling input should be determined considering the site-specific operating conditions, fluid characteristics, and types of failure and likelihood of environmental conditions. Once the risk levels are evaluated, sensitivity analysis for the key modeling inputs and parameters as given in this study should be used further to determine the risk management efforts.

In natural gas exploration and production industry, the risk management efforts including release event prevention and consequence mitigation are prioritized using the process risk assessment outputs which is based on the scenario-based consequence modeling and its likelihood. Facility siting and layout is a cost effective and powerful design step in process risk management (Nair and Salter, 2019a). The potential impact zone (hazardous distances) from facilities, pipelines and units forms key information in site selection and layout optimization in multi-million dollar projects. This challenge should be addressed by better understanding of the release, followed by the dispersion and its sensitivity to the consequence modeling inputs and parameters.

3.6. Discussion

There are several tools and methodologies available to determine the release and dispersion characteristics of the loss of containment and determine the hazardous level distances. Whichever approach is adopted, it should be used with an understanding of its range of validity, its limitations, the input data required, the sensitivity to the different input data, and how the results can be verified.

3.6.1. Findings

From the range of simulations (using HYSYS) and consequence modelling (using Canary), it was concluded that for a similar type of release event, the toxic hazard impact zone could be orders of magnitude different. Comparative study was carried out for eight different toxic natural gas compositions with H₂S concentration ranging from 2.6% to 29%. It was observed that the downwind distance to hazardous levels ranges from less than 50 ft to more than 5000 ft for a loss of containment from toxic natural gas pipeline transfer line. The range of results were obtained by varying input on the release (source term) conditions and certain environment conditions. From the parametric sensitivity analysis for a release event from a natural gas transfer pipeline at ground level using eight different compositions, the following are the observations and related guidance for toxic natural gas consequence modeling:

- Phase equilibrium properties of the release should be considered in determining the release phase as low temperature and high-pressure releases can have longer impact zone distances. Detailed review (prior to implementing risk mitigation) should be carried out for high pressure releases of compositions with >18 mol% H₂S & molar mass >29 lb/lbmol and for low temperature releases of compositions with molar mass >30 lb/lbmol.
- Downwind dispersion of toxic cloud is dependent on hole size, release rate and composition. The failure mechanism and related hole size for larger releases need to appropriately be determined. Dispersion from small hole releases is not sensitive to the composition of natural gas.
- Release rates and downwind dispersion are sensitive to low temperature for those compositions with >30 lb/lbmol. For such cases with significantly higher impact zone, further analysis should be carried out before implementing risk reduction measures.
- Downwind dispersion for high pressure releases is sensitive for compositions with greater than 18% H₂S content. For such cases with significantly higher impact zone, further analysis should be carried out before implementing risk reduction measures.
- The analysis implies that downwind dispersion is sensitive to the orientation of release; distance to H₂S concentration was note higher for composition S1 with 2.6% H₂S (highest molar mass and release rate) in comparison with the composition with higher H₂S compositions like S2 (8% H₂S) and S3 (10% H₂S). Release orientation also has significance in relation to the receptor of concern. So a site specific orientation shall be selected (not necessarily the worst case).
- Dispersion if natural gas with high toxic concentration has significant effect on wind speed and stability. For risk assessment purposes, it is advisable to have a range of stability and wind speed to represent the variations for 24 h and through the year (Pandya et al., 2012; US EPA, 2017).
- Variation in humidity has no significant impact on the downwind dispersion of toxic natural gas.

3.6.2. Further research

The statement is often made that natural gas is lighter than air and the property of a mixture is determined by the mathematical average of the properties of the individual constituents. Such mathematical boldness and inconsistency of thought is detrimental to safety and must be qualified (Speight, 2007). Process risk assessments for natural gas exploration and production projects where the content of H₂S in the

process stream is considerable have revealed that there is limited experimental data addressing releases of H₂S rich hydrocarbons (Nair and Wen, 2019b). It was observed that the computer tools can give substantially different results with respect to dispersion distances for the same accident scenario. The variations seem to be larger when the stagnant conditions are liquid or 2-phase (Nielsen et al., 2014). There are very limited, if any, experimental data to verify the accuracy of the models for H₂S rich natural gas (Nair and Wen, 2019b).

As underlined by the results and discussions based on this study simulations and literature review, the dispersion modeling is sensitive to a number of input and parameters. Sensitivity assessment for the key parameters is the recommended approach to overcome the uncertainty in the modeling (Pandya et al., 2013; US EPA, 2017). The literature review by Tauseef et al. reveals that there are weaknesses along with the strengths from list of software available for assessing consequences of process industry accidents (Tauseef et al., 2017). Computational Fluid Dynamics based codes and simulation software can model the complex thermodynamic processes during expansion and diffusion of H₂S rich natural gas. CFD can be used to effective study how the wind and environment can interfere with the gas dissipation in the air (Franklin et al., 2020). Further research is recommended to evaluate the CFD software options and determine appropriate solver and turbulence model for modeling H₂S rich natural gas. The study should also determine the key dispersion scenario inputs to be subjected for sensitivity assessment considering the highly computational power intensive simulations.

4. Concluding remarks

Numerical simulation of release and dispersion of natural gas provides an enhanced information on the potential impact zone which forms an essential part for risk-based decision making, especially in engineering projects and emergency planning. For toxic natural gas, with components like Hydrogen Sulfide (H₂S), the toxicity impact zone drives business decisions related to equipment design, facility siting, layout, land use planning and emergency response measures.

The study focused on potential accidental release from pipeline at ground level transferring toxic natural gas. Eight natural gas compositions were subjected to a range of release source terms and environmental parameter sensitivity analysis. The multi-component phase diagram was developed using HYSYS and release followed by and dispersion were estimated using Canary. Analysis was carried out for by changing one parameter at a time for release and environmental conditions.

The analysis concludes that the release and dispersion of toxic natural gas is significantly impacted by the natural gas composition and the H₂S content. As part of process risk assessments of toxic natural gas, detailed review (prior to implementing risk mitigation) should be carried out for H₂S rich natural gas (>18 mol% H₂S, molar mass >29 lb/lbmol) and for low temperature releases of compositions with molar mass >30 lb/lbmol. The study findings highlight the possibility of phase change depending on the composition and operating conditions and the significance of the use of a software with multicomponent model.

Incorrect selection of the modeling approach, input and environmental parameters could lead to an inaccurate consequence impact zone estimation which could result in disproportionate risk management efforts. This challenge can be addressed by selection of software models appropriate for the release scenarios and through sensitivity analysis of the modeling inputs and parameters. Further research using detailed physical modeling methods also suggested as a way forward to address the uncertainty in toxic natural gas dispersion modeling.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence

the work reported in this paper.

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