CHEMICAL ENGINEERING TRANSACTIONS

VOL. 77, 2019

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Genserik Reniers, Bruno Fabiano

ISBN 978-88-95608-74-7; **ISSN** 2283-9216

DOI: 10.3303/CET1977060

Uncertainties in Sour Natural Gas Dispersion Modelling

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Unplanned and uncontrolled releases of hazardous materials could result in major casualties and environment impact. Natural gas (sour) containing significant amounts of hydrogen sulfide is toxic, flammable and corrosive. Incidents like 2003 Kaixian blowout ("12.23 disaster") and 2015 Saskatchewan in Oil & Gas industry highlight the significance of conducting appropriate technical (safety) risk assessments and exercising effective risk management. It is estimated that for 90% of accidental releases of sour gas during pipeline transfer results toxic impacts as typical releases will not get immediately ignited. Lack of adequate information of the hazards and the lack of realistic estimate of the hydrogen sulfide toxic exposure zone are the main challenges in addressing the risk to public from sour natural gas.
The challenge risk analysts come across is the lack of guidance on appropriate tool and methodology to estimate the toxic impact zone following an accidental loss of containment. Dispersion following accidental release of high pressure and high flow rate sour gas in complex terrain should take account of multicomponent thermodynamics, terrain effect and the phase transitions. For selecting processing sites, pipeline routes etc., stakeholders require convincing results addressing the uncertainties. Simple correlation like Gaussian model alone is not considered as suitable and appropriate.
This paper is based on the academic research conducted to overcome the uncertainties in sour gas dispersion modelling. The focus of this research is on the dispersion following an accidental release from sour natural gas pipeline. The expansion following release and the initial air entrainment will be estimated to determine a range of cloud behaviour. Based on the sensitivity analysis, this paper provides guidance on the natural gas composition and the source term characteristics to define and select the appropriate dispersion phenomenon. The results and analysis will minimize the knowledge gap/uncertainty with the consequence calculations by identifying the key assumptions and parameters that should be put through sensitivity analysis.

1. Introduction

Natural gas is a clean and naturally occurring hydrocarbon gas mixture which is an efficient source of energy. Natural gas consists primarily of methane (molecular mass 16 g/mol, lighter than air) 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 (Kelly B.T. et.al. 2011). Natural gas is usually considered 'sour' if there are more than 5.7 milligrams of Hydrogen Sulfide (H_2S) per cubic meter of natural gas, which is equivalent to 4 ppm by volume (approximately) under standard temperature and pressure (Speight, 2007). H_2S is highly toxic (fatal effects at low concentration), extremely flammable and corrosive. The molecular mass of H_2S is 34.1 g/mol, and it is thus slightly heavier than air (29 g/mol) at standard conditions.
Natural gas is commonly transported using a pipeline (Deng Y. et. al., 2018) and loss of containment from the gas pipeline occurs due to integrity degradation and external factors like earthquakes, human activities. Major incidents involving loss of containment of sour natural gas, like 1992 Gezi (Zhao 48# well) and 2003 Kaixian blowout (the "*12.23*" disaster) illustrates the serious threat from handling and transporting sour gas. In their paper, Bariha et.al (Bariha N. et. al., 2016) reported that out of 185 accidents involving natural gas, the pipeline accidents accounted for 127 and the most frequent accident were caused by mechanical failure (fatigue, creep, brittle fracture, and corrosion) of the pipelines or due to significant changes to the surrounding environment. 90% of sour natural gas releases could result in toxic cloud dispersion with potential impacts

Paper Received: 2 December 2018; Revised: 30 May 2019; Accepted: 19 June 2019

Please cite this article as: Nelly S., Wen J., 2019, Uncertainties in Sour Natural Gas Dispersion Modelling, Chemical Engineering Transactions, 77, 355-360 DOI:10.3303/CET1977060

(Muhlbauer W.K., 2004). Predictive risk assessments are carried out to determine the extent of hazardous level distances (impact zone) and how frequently such events can happen.

2. Methodology

2.1 Description of the problem and the approach

Consequence assessment consists of the assumptions and calculations used to predict the potential impacts of an accidental release of hazardous material; this includes the estimation of release/discharge rate, initial mixing, dispersion and phase changes. As per US EPA guidance, in general, consequence modelling approaches can be clustered into:

- Simple correlation or formulae, e.g. Gaussian: if probabilistic approximation is sufficient;
- General purpose integral tools: for dense gas, jet like dispersion, neutral, then Gaussian;
- Computational Fluid Dynamics (CFD) or Three dimensional (3D): deterministic answers
- Experiments, wind tunnel and field testing.

In this paper, sour natural gas release from of a pipeline transporting sour natural gas from reservoirs (gas fields) to treatment/processing plants is considered. The treatment plant (usually common for several gas fields) could be at a distance such that the pipeline has to be routed through populated areas and through areas without continuous monitoring for any leaks. Methane (CH_4) and H_2S at different compositions will be evaluated in this study. A continuous high pressure dense natural gas leak from a typical 6” pipeline is considered as the scenario of concern. This scenario is modelled using a general-purpose tool to estimate the downwind distance for the hazardous region of concern. The key assumptions and parameters of interest is determined through sensitivity analysis.

2.2 ALOHA model

The Aerial Locations of Hazardous Atmospheres (ALOHA) model is used to estimate the release and dispersion of CH_4 and H_2S. 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. ALOHA can predict the atmospheric dispersion rate and direction of vapours and can also generate a visual representation of the plume created by the chemical release. The tool selects Gaussian (buoyant) or dense models depending on the properties of the released material.

2.3 HYSYS model

Aspen’s HYSYS is a chemical process simulator used to mathematically model chemical processes, from unit operations to full chemical plants and refineries. HYSYS modelling is used to estimate the phase equilibrium of natural gas for different H_2S compositions.

2.4 Release and dispersion

The process of gas releases from pipeline leak scenario can be divided into three stages, namely the discharge, expand and dispersion as illustrated in Figure 1.

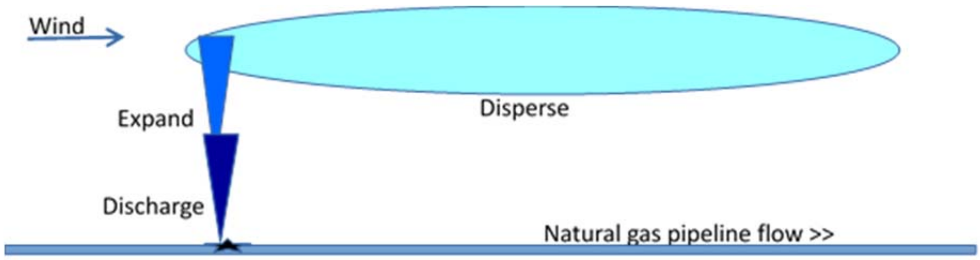

Figure 1: Release and dispersion scenario

Release: The influencing conditions and the parameters that determine the phase of release and the characteristics of the fluid near the release source and till the point at which dispersion kicks-in usually dependent on the composition of the discharged material, the rate or quantity of the discharge and the ambient conditions (Fontaine, D.J. and Hall, M.E. Jr., 1991).

Dispersion: The dispersion mechanisms could include turbulent jet, slumping dense plume (for dense gases) followed by passive dispersion (dependent of the turbulence). As per US GAO (GAO, 2012), several factors that could influence the dispersion can be classified as (i) Physical process, (ii) Transport by wind and heat convection and (iii) Turbulent diffusion (random mixing of air mass); similarly the factors that could guide the dispersion can be classified as (i) Source / release conditions, (ii) Weather conditions near the source and along the dispersion, (iii) Thermodynamic properties of the dispersed products and topography (site, deposition, surface roughness).

2.5 Simulation cases and criteria

The simulation cases are run for single phase, continuous long-term release from transfer pipeline at constant pressures for the Pasquill-Gifford atmospheric stability category F and for wind speed 1 m/s at ambient temperature 8 ^{o}C. Using the calculated concentration distribution for the set of input and assumptions, the hazardous distance can be obtained for the lower explosive limit (LEL) levels for CH_4 and toxic exposure levels for H_2S. The distribution of concentration could vary in areas of actual vapour cloud and generally a lower level of concentration is set as criteria. In this paper three hazardous concentration criteria levels are set and the threshold criteria values for CH_4 and H_2S as given in Table 1.

Table 1: Hazardous levels of pipeline release of sour natural gas

Component	Material properties	Accidental consequence	Level-3	Level-2	Level-1
Methane (CH_4) CAS Number: 74-82-8	Molecular mass: 16 g/mol; Boiling point: -161 ^{o}C; Gas density: 0.678 kg/m^3	Flash fire (flammable vapour cloud distance)	LEL (50,000 ppm)	60% LEL	10% LEL
Hydrogen sulfide (H_2S) CAS Number: 7783-6-4	Molecular mass: 34 g/mol; Boiling point: -60.3 ^{o}C; Gas density: 1.45 kg/m^3	Toxic concentrations of significance	400 ppm; loss of consciousness after short exposures, potential for respiratory arrest	200 ppm; potential for pulmonary edema after 20 minutes	100 ppm (IDLH); coughing, headache, dizziness; loss of sense of smell in minutes

The source release parameters (Table 2) is designed based on the conditions of natural gas pipeline similar to the conditions for Kaixian, Kai County, China. The toxic cloud hazardous level distance estimation is validated against the actual monitored values from Kaixian (1.24) disaster given in the case study by Qingchun M and Laibin Z (2011).

3. Numerical methods, results and discussion

To study the effect of the input factors on the accident consequences, a series of release scenarios were designed and calculated, with conditions close to Kaixian “12.23” incident. The considered base case scenario and the sensitivities is simulated in ALOHA and the results are analysed to determine the key input parameters of significance. Input parameters that does not have major impact in the estimation of hazardous level distance is screened out from further sensitivity and detailed analysis.

3.1 ALOHA results

The release and dispersion modelling using ALOHA is limited to one component at a time. Though natural gas consists of a range of constituents, for this paper, modelling and results for two components only were evaluated. Release and dispersion modelling was carried out for 100% CH_4 and 100% H_2S as separate cases. The input data for the base case and sensitivity cases for ALOHA are listed in table 2:

Table 2: Input for base case and sensitivities

Description	Release conditions	Atmospheric stability and wind speed	Ambient temperature and humidity	Inversion layer height and surface roughness
Base case	Release from 6” pipeline at ground level; continuous release from rupture in vertical orientation at 30 barg (CH_4); at 12.4 barg (H_2S)	F stability (typical night time / stable); 1 m/s wind speed	8 ^{o}C; 50% humidity	No specific inversion height (end of momentum jet); Terrain similar to open country (minimum turbulence from obstacles)
Sensitivity	Release rate similar to Kaixian blowout - 100 kg/s	D stability (typical day time /neutral); 5 m/s	25 ^{o}C; 50% humidity	Inversion at 1000 m, 100 m, 15 m; Terrain to represent urban or forest

Inversion refers to a layer of air (change in temperature at altitude) that resists upward motion of air. This phenomenon (entrapment) could impact the distance compared to free dispersion. A representative illustration of un-ignited gas cloud to downwind direction for three concentration levels of interest is given in figure 2a (CH_4) and figure 2b (H_2S).

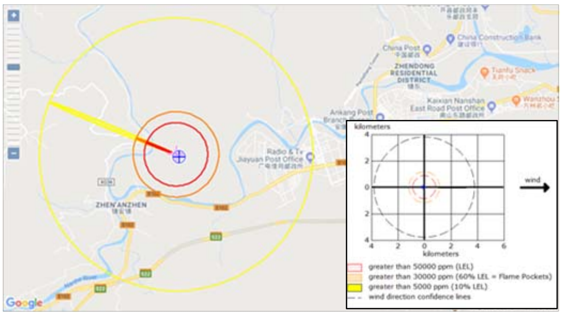

Figure 2a: Methane flammable cloud dispersion

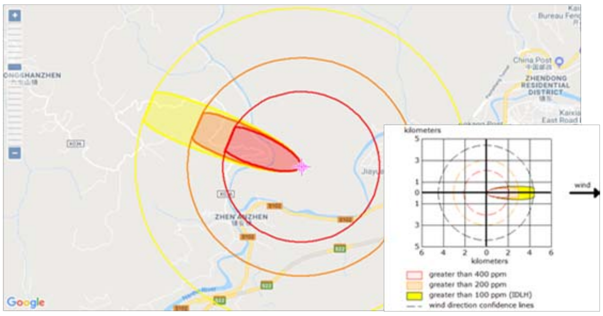

Figure 2b: Hydrogen sulfide toxic cloud dispersion

The figures indicate that the hazardous level distance and the area under impact for toxic consequences from H_2S dispersion (400 ppm) is longer and wider than flammable zone (LEL). It is noted that in ALOHA Gaussian (passive dispersion) model was run for CH_4 and heavy gas (gravity slumping) model was run for H_2S based on the release characteristics and the density of the released material.
The hazardous level distances for the same set of discharge conditions is sensitive to dispersion parameters and as a result the cloud dispersion can vary significantly. A comparison of the results from the sensitivity analysis for the input parameters listed in Table 2 is given in figure 3.

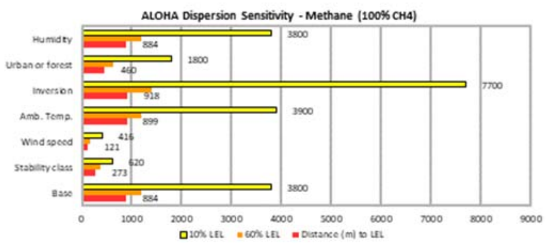

Figure 3a: Methane dispersion - sensitivity

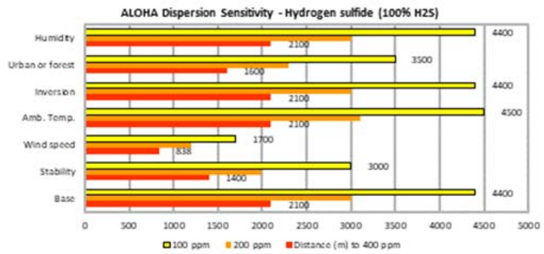

Figure 3b: Hydrogen sulfide dispersion - sensitivity

It is observed that the hazardous level distance (LEL) for lighter gas (CH_4) ranges from 120 m to 920 m and for heavier gas (H_2S) the 400 ppm distance ranges from 840 m to 2100 m. By analysis of the ALOHA dispersion results, following conclusions were arrived:

1. Dispersion of CH_4 and H_2S are not significantly sensitive to the changes in humidity and ambient temperature.
2. H_2S (heavier gas) is not sensitive to inversion layer height, but, CH_4 (lighter than air) is very sensitive to inversion layer height and it is observed that the downwind distance can be longer (see inversion Figure 3a) if the discharged material (momentum jet) reaches the inversion layer (lower inversion levels heights are likely during calm night time conditions).
3. Both lighter and denser gas cloud dispersion is sensitive to the turbulence related parameters, i.e. stability class, wind speed and surface roughness.

The cloud dispersion behaviour can be categorised to lighter than air clouds (buoyant gas) and heavier than air clouds. ALOHA modelling can be performed for a single component only, but natural gas exists as multi-component. In order to determine the appropriate modelling parameters and EOS, risk analysts need to determine the characteristic of the released multi-component material. The density of the material is key factor for the selection of the dispersion modelling approach.

3.2 Validation

It is not feasible to conduct a field test of the dispersion of natural gas with high H_2S content from high pressure pipeline transfer due to the enormous toxic impacts (danger to public and environment). Hazardous level distances estimated by Qingchun M and Laibin Z (2011) using ANSYS FLUENT based on the impact from Kaixian "12.23" incident is used for comparison to the ALOHA predicted H_2S dispersion results at similar release and atmospheric conditions. The post-incident field data indicates nearly 100% fatalities within 200 – 500 m (Xiaoyan village) and the longest distance noted for death as 1200 m. The prediction results of downwind hazardous level distances close to ground level are not in agreement with the available incident data; FLUENT estimated 200 ppm reaching 1270 m whereas ALOHA estimated 200 ppm reaching 2000 m. A summary of the comparison is given in Table 3.

Table 3: Hazardous level distance of hydrogen sulfide dispersion

Case description	Results to H_2S concentration	400 ppm	200 ppm	100 ppm
FLUENT, Kaixian 16H well blowout; natural gas	Mass flow at 98.8 kg/s; 16% H_2S (Mass%: 68% CH_4 and 7% CO_2)	0.623 km	1.271 km	2.15 km
ALOHA, this study; 100% H_2S	Mass flow at 15.4 kg/s representing 16% mass flow rate of H_2S in natural gas.	1.3 m	2.0 km	3.2 km

Parameters were changed in ALOHA to calibrate the terrain and weather sensitivity. However, the study shows that a simple tool like ALOHA, designed for emergency responses with conservative results, is not suitable for detailed engineering and emergency response planning considering weather and terrain effects.

The FLUENT simulation results of the gas (with high H_2S) dispersion after the well blowout shown the characteristics of heavy gas. The incident and the case study also confirm that the high-sulfur gas is affected by terrain, wind speed and move quickly along valleys (Qingchun M and Laibin Z, 2011). Further analysis was carried out to determine the concentration of H_2S (sourness) in natural gas that initiates the dense-gas behaviour.

3.3 HYSYS results

HYSYS modelling was carried out to estimate the phase equilibrium of natural gas for different H_2S compositions at 30 barg. Natural gas (a non-ideal gas) obey the modified gas law.

$$PV = nZRT \qquad (1)$$

Where; P = pressure, V = volume; T = absolute temperature (^oK); Z = compressibility; n = number of kilo-moles of the gas; R = gas constant.

The compressibility factor distinguishes natural gas from an ideal gas. Pipelines may operate at very high pressure (above 70 barg) to keep the gas in the dense phase, thus preventing condensation and two-phase flow. Peng-Robinson Equation of State (EOS), the model for non-ideal vapor phase, was selected in HYSYS to estimate the phase equilibrium. The results from the simulations are summarized in figure 4.

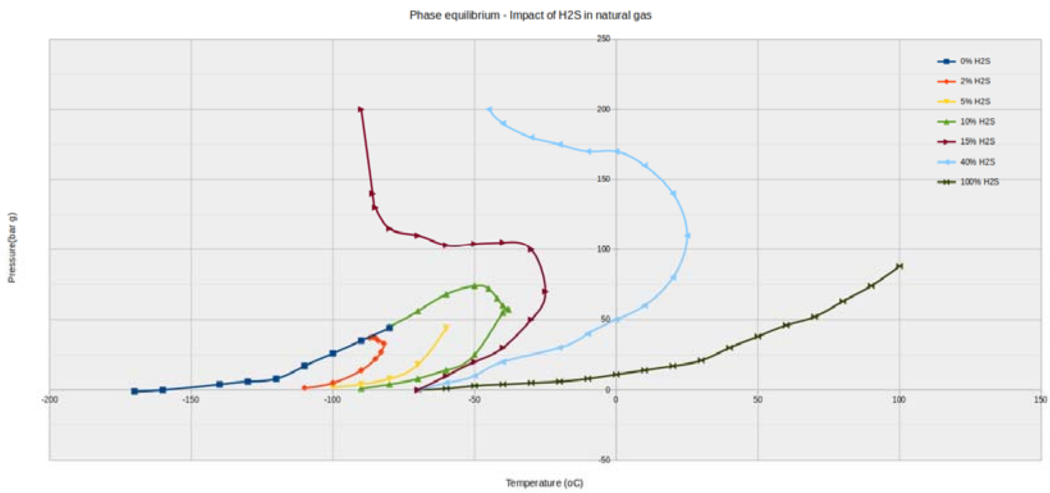

Figure 4: Phase equilibrium – impact of H_2S concentration in natural gas (CH_4)

The phase equilibrium curves from 0% H_2S (i.e. 100% CH_4) to 100% H_2S (i.e. 0% CH_4) is plotted. It is observed that the lighter gas behaviour of the natural gas is followed for lower concentration of H_2S; but, starts to change when the H_2S concentration exceeds 10% and behaves more like dense gas when concentration exceeds 15%. Calculation results from the study by Nilsen et. al. (2014) for different sour gas compositions also concludes on a similar finding that significant differences in the discharge and dispersion for the combinations of EOS and expansion methods for varying concentration of sour components in natural gas.

3.4 Summary and further research

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.

The statement is often made that natural gas is lighter than air and the properties of a mixture is determined by the mathematical average of the properties of the individual constituents. Such mathematical bravado and inconsistency of thought is detrimental to safety and must be qualified (Speight, 2011 P 71). During expansion from elevated pressure, released H_2S will be colder and thus even heavier than air close to the release source with a high potential to accumulate in low-lying areas. CH_4 dissipates readily into the air, whereas the other hydrocarbon constituents (heavier than air) could accumulate or pool at ground level and pose threat to public and environment.

Safety analyses for projects where the content of H_2S in the process stream is considerable have revealed that there is limited experimental data addressing releases of H_2S rich hydrocarbons. 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 (Nilsen et. al. 2014). The literature review and simulations indicate that there exist so called simple models and algorithms cannot adequately consider H_2S specific properties in natural gas dispersion. Also, there are very limited, if any, experimental data to verify the accuracy of the models. Sensitivity modelling for the key parameters is the suggested approach to overcome this challenge. It also became clear that CFD codes can model the complex thermodynamic processes during expansion and diffusion of H_2S rich hydrocarbons. Further research is recommended to evaluate the CFD modelling parameters that are key such that sensitivity analysis need to be performed.

4. Conclusions

Numerical simulation provides an enhanced information on gas dispersion which forms essential part for risk-based decision making, especially in engineering projects and emergency planning. The paper focused on the dispersion following an accidental release from sour natural gas pipeline. The discharge and dispersion were estimated using ALOHA to determine the cloud behaviour. The methodology and results were validated against the post-event data (Kaixian “12.23” incident) based simulations using FLUENT.

During a pipeline rupture or major leak, depending on the particular gaseous mixture properties, and ambient conditions, the sour gas cloud from a release may 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 (e.g. wind speed).

According to this study, the key physical parameters that should be considered for sensitivity modelling are weather stability, wind speed and surface roughness (terrain effects). Natural gas dispersion is less sensitive to the humidity and ambient temperature changes. The discharge and dispersion of natural gas should be based on the dominant characteristics (lighter or dense-gas) of the mixture. Further analysis showed that if the fraction of H_2S in sour natural gas is larger than 10%, then heavy gas behaviours will be prominent. The scarcity of experimental data for H_2S rich fluids and variations in results in calculations give reasons to implement results from risk analysis with caution. Sensitivity modelling for the key parameters is the suggested approach to overcome this challenge.

References

Bariha N., Mishra I.M., Srivastava V.C., 2016, Hazard analysis of failure of natural gas and petroleum pipelines, Journal of loss prevention in process industries, 40, P217-226

Deng Y., Hu H., Sun D., Hou L., Liang Y., 2018, A method for simulating the release of natural gas from the rupture of high-pressure pipelines in any terrain, Journal of Hazardous Materials, 342, P418-428

Fontaine, D.J. and Hall, M.E. Jr., 1991, Dispersion modelling of gas releases on Offshore platforms, SPE 23288

GAO, 2012, Pipeline Safety - collecting Data and Sharing Information on Federally Unregulated Gathering Pipelines Could Help Enhance Safety, The US Governmental Accountability Office, GAO-12-388

Kelley, B.T., Valencia, J.A., Northrop, P.S. and Mart, C.J., 2011, Controlled free zone for developing sour gas reserves, Energy Podia 4, P824-829

Muhlbauer W.K., 2004, Pipeline risk management manual ideas, techniques and resources, 3rd Edition, ISBN: 0-7506-7579-9, 14/327 – 328

Nilsen S., Hoiset S., Salaun N., 2014, Improving safety risk tools for accidental fluid releases with high H2S concentrations, Abu Dhabi International Petroleum Exhibition and Conference, SPE-171809-MS

Qingchun, Ma and Laibin Zhang, 2011, CFD simulation study on gas dispersion for risk assessment: A case study of sour gas well blowout, Safety Science 49, P1289–1295

Speight, J. G., 2007, Natural Gas – A basic handbook, Gulf publishing company, ISBN 1-933762-14-4

US EPA, 2005, Appendix W to 40 CFD Part 51: Guideline on Air Quality Models, Alternate models recognized for specialized applications, www3.epa.gov/scram001/guidance/guide/appw_99.pdf