

CFD-based Multiphysics Simulation of Toxic Gas Emissions from Industrial Storage

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Abstract

Almost all industrial processes produce exhaust and use chemicals potentially harmful to humans. This is even more applicable for chemical industries whose primary raw materials and products may be detrimental to people's health. As a result, people working or living nearby chemical industrial clusters remain in an intensified state of risk for prolonged exposure and accidental catastrophic chemical leakage events. Sudden accidental release of chemicals needs to be considered for industrial design and planning. Exposure to toxic chemicals can cause severe health outcomes and, in some cases, even death as well as damage to surrounding wildlife, vegetation and entire environment. The stakes are quite high when it comes to planning and response to such emergency scenarios. Mathematical simulation modeling of sudden catastrophic chemical releases can provide insight into dispersion trends depending on various chemical properties, ambient conditions and terrain characteristics. Proper precautions and emergency responses can be effectively planned and implemented based on the comprehensive understanding gained from such simulations.

In this work finite element models of an industrial chemical storage unit releasing its content on the surrounding environment were developed. It was developed using the COMSOL Multiphysics® version 6.2. The developed models were executed on both workstation and supercomputer depending on the domain size and the simulation time. Compared to the entire geometry of the model, small element size was used to obtain a high-resolution model which provided detailed and accurate simulation of a hypothetical catastrophic chemical release. The diffusion and convection of the released chemical are the prevailing driving mechanism of transport. The dispersion trend was estimated by using Fick's 2nd law of diffusion integrated with convection by velocity field of ambient air. A turbulent flow model was employed to simulate the wind velocity field, with altitudinal wind speed variation systematically incorporated into the analysis. Physical, thermodynamic and transport properties of the chemical were used to estimate the leakage flow properties. The effects of varying terrain conditions (plain terrain and terrain with varying number of obstacles) on the dispersion of the chemical were studied. Velocity field for different wind speeds have been calculated by using compressible form of the Navier-Stokes and continuity equations. Varying wind speeds' effect on the dispersion trends were observed over time. The influence of velocity on the local concentration buildup of the released species was interpreted based on the fluid mechanics principles and phenomena.

Keywords: Toxic Release Dispersion, CFD, FEA, Diffusion

Introduction

Chemical industries are a crucial part of the productive industrial base of USA. It sits upstream of many other industries that produce enormous physical goods and contribute billions to the GDP and its importance for national security cannot be overstated. The unintended release of toxic gases from industrial facilities, chemical storage sites, or transportation incidents poses significant hazards to human health, environmental integrity, and public safety. Furthermore, legal liability must be understood as an umbrella category of risks with multiple faces. Physical harm posed by an accidental chemical release can range from a minor

temporary discomfort to a permanent health damage, or a lifelong chronic health issue to even death. Accidental chemical release incidents necessitate safeguarding of active workers along with evacuation of nearby communities.

1,3-Butadiene is one of the most aggressive chemicals in terms of toxicity to human health. It is classified as a human carcinogen of developing leukemia and other cancers affecting the blood and lymph system.¹ This volatile organic compound is widely used in petrochemical industries, especially in polymer, and rubber processing facilities.

The velocity field of wind and dispersed gas varies significantly in local level throughout the exposure domain due to pressure difference by the obstacles and surfaces. Afterwards, the dispersion trend of the released gas is directly influenced by the velocity field. A Computational Fluid Dynamics (CFD) based simulation offers transient solutions of

dispersion with spatial details in case of complex or obstructed terrain.

EPA ALOHA is a popular tool for estimating the threat zone resulting from any chemical release accidents. However, ALOHA does not provide instantaneous concentration field for the released gas. The heavy gas dispersion model of ALOHA based on integral conservation laws provides cumulative estimation of the hazard/consequences by averaging the physical properties over a bulk volume in a 1-hr window. Whereas CFD analysis considers spatial and temporal resolution of the system. Furthermore, spatial distribution in all 3 dimensions can be estimated by a 3D CFD simulation which is not available for ALOHA. In this research, a simulation based on CFD was carried out for hypothetical accidental release scenarios of 1,3-butadiene vapor. The concentration profile and history of 1,3-butadiene vapor was analyzed in local and temporal resolution. Effect of obstacles and different wind speeds were discussed in context of fluid dynamics phenomena.

Governing Equations

COMSOL Multiphysics® version 6.2 was used to perform the release gas simulation. Turbulent flow principle was used to calculate the velocity field of the ambient air. Using the result of velocity field, concentration of the dispersed chemical was calculated by using Fick's 2nd law of diffusion. The k - ϵ Turbulent Flow Model from Fluid Flow module and Transport of Diluted Species from Chemical Engineering module were used in this work. The subsequent calculation procedures applied in this simulation are well posed as described in the following subsections.

Fluid Flow

The velocity field of wind and released gas was calculated by using the k - ϵ Turbulent Flow model. The interface uses Reynolds-Averaged Navier–Stokes (RANS) equation for conservation of momentum (eq 1) and continuity equation (eq 2) to account for turbulence in case of high Reynolds number fluid flow.

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + (\mu + \mu_T)(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} \quad (1)$$

$$\rho \nabla \cdot (\mathbf{u}) = 0 \quad (2)$$

k - ϵ Turbulent Flow Model was used to account the turbulence of the wind flow. Two turbulent variables such as turbulent kinetic energy, k and dissipation rate of turbulent kinetic energy, ϵ were solved in the time-dependent solver with eq 3 and eq 4.

$$\rho \frac{\partial k}{\partial t} + \rho(\mathbf{u} \cdot \nabla) k = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right] + P_k - \rho \epsilon \quad (3)$$

$$\rho \frac{\partial \epsilon}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \epsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_\epsilon} \right) \nabla \epsilon \right] + C_{\epsilon 1} \frac{\epsilon}{k} P_k - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} \quad (4)$$

where C_μ , $C_{\epsilon 1}$, $C_{\epsilon 2}$, σ_k and σ_ϵ are empirical constants used in this model. The values of the constants used in this study were as follows²:

$$C_\mu = 0.09, C_{\epsilon 1} = 1.44, C_{\epsilon 2} = 1.92, \sigma_k = 1, \sigma_\epsilon = 1.3.$$

P_k is the production of turbulence kinetic energy due to velocity gradient and eddy formation can be estimated by the eq 5 considering the fluid is compressible.

$$P_k = \mu_T [\nabla \mathbf{u} : (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u})^2] - \frac{2}{3} \rho k \nabla \cdot \mathbf{u} \quad (5)$$

k - ϵ turbulence model estimates the turbulent viscosity μ_T from eq 6 correlated with turbulent kinetic energy and dissipation rate.

$$\mu_T = \rho C_\mu \frac{k^2}{\epsilon} \quad (6)$$

Mass Transport

The transport of the released species through the ambient air was simulated by using Fick's 2nd law of diffusion. The transports by diffusion and convection were integrated into the equation as described in eq 7 and eq 8.

$$\frac{\partial c_i}{\partial t} + \nabla \cdot J_i + \mathbf{u} \cdot \nabla c_i = R_i \quad (7)$$

$$J_i = -D_i \nabla c_i \quad (8)$$

where

c_i = concentration of the species

J_i = mass flux

$\mathbf{u}$ = velocity field

D_i = diffusion coefficient

R_i = reaction source

The velocity field calculated in the Fluid Flow was used as values of $\mathbf{u}$ in eq 7.

Discharge Flow of the Leakage

The pressure inside the storage tank was assumed to be at a constant of 2.7 atm³, the vapor pressure of liquid 1,3-butadiene at the studies temperature (25 °C) since the partially-filled liquid storage tank is under vapor-liquid equilibrium.

The discharge flow rate of the gas was calculated by using the following eq 9.⁴

$$\dot{Q} = C_0 A P_1 \sqrt{\left(\frac{2g_c M_w}{R T_0} \frac{\gamma}{\gamma - 1} \left[\left(\frac{P_{down}}{P_1} \right)^{\frac{2}{\gamma}} - \left(\frac{P_{down}}{P_1} \right)^{\frac{(\gamma - 1)}{\gamma}} \right] \right)} \quad (9)$$

where

$\dot{Q}$ = mass flowrate through the leak in kg/s

C_0 = discharge coefficient (unitless)

A = area of leakage in m²

P_1 = pressure inside the tank in kPa
 P_{down} = downstream pressure in kPa (1 atm in this study)
 R = gas constant in $\text{J K}^{-1} \text{mol}^{-1}$
 g_c = unit conversion factor
 M_w = molecular weight of the gas
 T_0 = temperature inside the tank
 γ = ratio of heat capacity

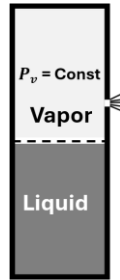


Figure 1. Visual presentation of half-filled liquid storage tank.

Model Set Up

1,3- Butadiene was chosen for the toxic gas dispersion study since it is one of the common toxic pollutants released in petrochemical, plastic and rubber industries. This chemical is classified as carcinogenic by inhalation for humans by US EPA. The toxicity level of 1,3- Butadiene in brief is listed in Table 1.

Table 1. Advisory/regulatory critical concentration levels of 1,3 Butadiene.⁵⁻⁸

Regulatory/Advisory Level	Critical Conc. Level (ppmv)	Exposure Duration	Health Effect Endpoint
RfC	0.001	Chronic Exposure	US EPA
OSHA PEL ^a	1	8-hr TWA (Time-weighted average)	Carcinogen; lowest feasible control level for workers
OSHA STEL ^b	5	15-min STEL	Short-term carcinogen/acute irritant protection
AIHA ERPG-1 ^c	10	1 hour	Mild, transient health effects, detectable odor
AIHA ERPG-2 ^c	200	1 hour	Irreversible of serious health effects

Regulatory/Advisory Level	Critical Conc. Level (ppmv)	Exposure Duration	Health Effect Endpoint
AIHA ERPG-2 ^c (2016 Edition with less conservative approach)	500	1 hour	Irreversible of serious health effects
NIOSH IDLH ^d	2000	30 min	Life-threatening effects

^aOccupational Safety & Health Administration's permissible exposure limit

^bOccupational Safety & Health Administration's short-term exposure limit

^cAmerican Industrial Hygiene Association's emergency response planning guideline

^dNational Institute of Occupational Safety & Health's immediately dangerous to life or health concentration

Two different accidental release scenarios were considered in the study.

Case 1: 1,3-Butadiene released through a 1-cm diameter leakage from a 66,000 US gallon main storage tank which was 50% filled with liquid 1,3-butadiene.

Case 2: 1,3-Butadiene released through a 2-cm diameter leakage from a 12,000 US gallon intermediate bullet storage tank which was 50% filled with liquid 1,3-butadiene. The leakage velocity was assumed to be 50 m/s in this case.

Two different wind speeds, 5 m/s and 10 m/s were applied in both cases.

Geometry and Mesh

A three-dimensional computational domain with dimensions 150 m (length) $\times$ 50 m (width) $\times$ 50 m (height) was considered for the CFD simulation for Case 1. The storage tank (5 m $\times$ 5 m $\times$ 10 m) was placed at $x = 20$ m, positioned along the centerline of the domain. A circular emission source with diameter 1 cm positioned at an elevation of 6 m above ground was configured on the leeward vertical face of the storage tank. A 5 m $\times$ 5 m $\times$ 10 m obstacle at the downward side of the tank was placed at $x = 75$ m in the geometry of obstructed terrain. The geometry of both plain and obstructed terrains is depicted in Figure 2.

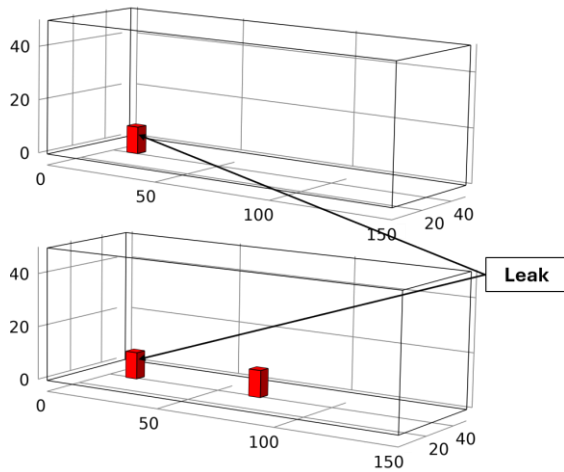


Figure 2. Geometry of plain (Left) and obstructed terrain (Right) of Case 1.

Fine mesh with free triangular mesh element was implemented on and around the leakage hole. Unstructured free tetrahedral mesh was used in mesh control domain adjacent to the leak and structured swept mesh was used in the remaining domain of the geometry of Case 1. The mesh near the leak and whole domain for Case 1 are shown in Figure 3 and Figure 4.

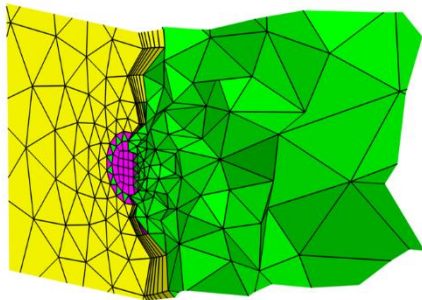


Figure 3. Mesh around the leak (Case 1).

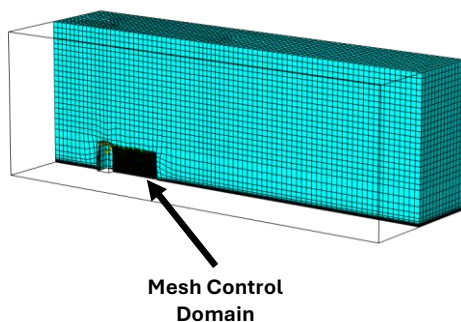


Figure 4. Mesh in the whole domain of Case 1.

Initial and Boundary Conditions

The wind velocity field was calculated in a stationary solver at the first step of the simulation procedure. The result of the stationary velocity field of the wind was used the initial condition for the time dependent solver for the transient analysis of the velocity of wind and released gas and the concentration of the species afterwards. The initial velocity field of wind for both cases is presented in Figure 5 through Figure 8.

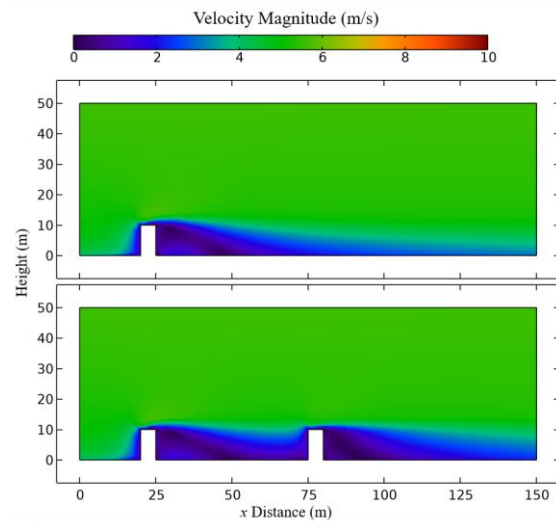


Figure 5. Velocity profile of 5 m/s ambient wind speed along x-z plane through centerline ($y = 25$ m) in plain terrain (Top) and obstructed terrain (Bottom) of Case 1.

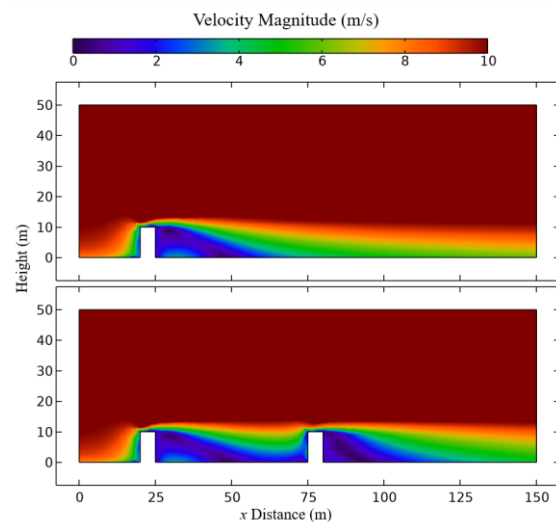


Figure 6. Velocity profile of 10 m/s ambient wind speed along x-z plane through centerline ($y = 25$ m) in plain terrain (Top) and obstructed terrain (Bottom) of Case 1.

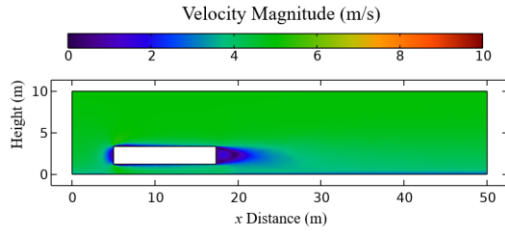


Figure 7. Velocity profile of 5 m/s ambient wind speed along x-z plane through centerline ($y = 10$ m) of the domain of Case 2.

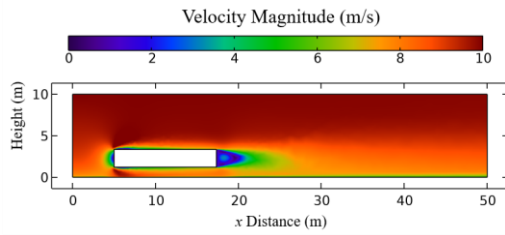


Figure 8. Velocity profile of 10 m/s ambient wind speed along x-z plane through centerline ($y = 10$ m) of the domain of Case 2.

Boundary conditions applied on all the boundaries of the domain for both cases were chosen for the simulation as described in Figure 9 and Figure 10 for both cases.

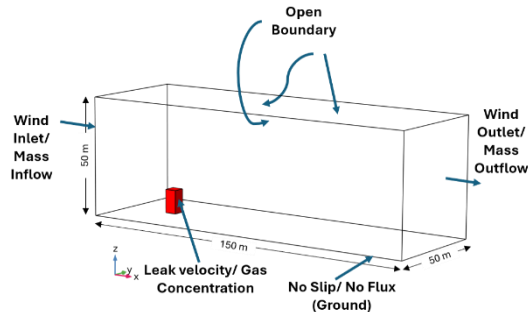


Figure 9. Boundary conditions for fluid flow and mass transport interfaces in the domain for Case 1.

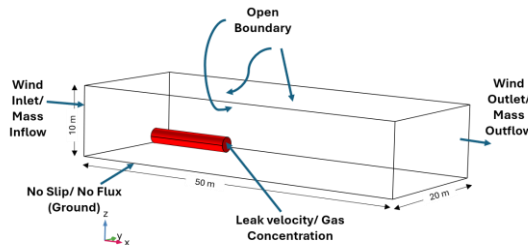


Figure 10. Boundary conditions for fluid flow and mass transport interfaces in the domain for Case 2.

The velocity of the released gas through the leakage was calculated by using eq 10 in the study of Case 1 scenario.

$$u_t = \sqrt{\frac{2g_c C_0^2 RT_0}{M} \times \frac{\gamma}{\gamma-1} \times \left[1 - \left(\frac{P_{down}}{P_1} \right)^{\frac{\gamma-1}{\gamma}} \right]} \quad (10)$$

In the scenario of Case 2, the velocity of released gas through the leakage was assumed to be 50 m/s.

It was assumed that pure 1,3-butadiene vapor was leaking out of the tank. The concentration of the released gas was calculated by using the ideal gas law assuming the tank pressure was constant due to vapor-liquid equilibrium inside the tank.

Results and Discussion

The CFD based simulation captured the detailed effect of ambient velocity field on the concentration field of the dispersed gas in this research. The structure of the exposure terrain as well as wind speed showed notable influence on the distribution of the gas in the scenario of Case 1. The obstacle exerted blocking effect on the dispersion. The surface plot on x-z plane through the centerline of the domain ($y = 25$ m) in different terrain structures and wind speeds is presented in Figure 11. Under 5 m/s wind speed, the trailing edge of the plume reached $x = 100$ m in plain terrain after 30 s of the release. On the other hand, the obstacle made the plume confined around the obstacle ($x = 80$ m) in the obstructed terrain after 30 s.

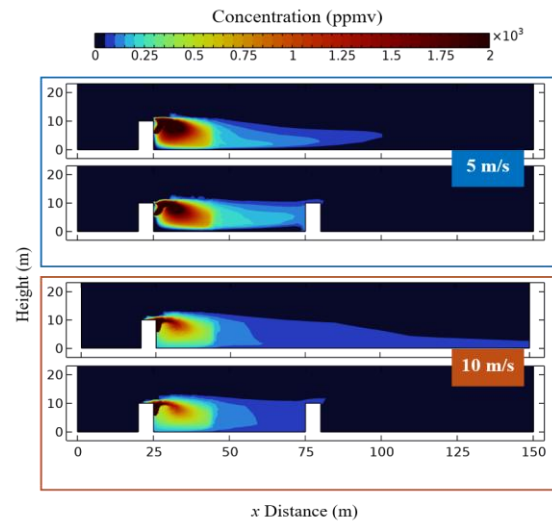


Figure 11. Concentration profile of 1,3-Butadiene after 30 s along x-z plane through the centerline ($y = 25$ m) for Case 1.

A 10 m/s wind speed facilitated enhanced the horizontal transport of the gas, therefore the end of the plume reached a longer distance compared to that when a 5 m/s wind speed was applied. Figure 11 shows the dark blue color band of low concentration (50–100 ppmv) reached $x = 100$ m in plain terrain at 5 m/s wind speed, while the same concentration band already reached $x = 150$ m at

the same time under a 10 m/s wind speed in plain terrain. A 5 m/s wind speed yielded stratified layers of high concentration zones near the ground to an extended distance. For instance, the color band of concentration 100–150 ppmv reached $x = 79$ m at 5 m/s wind speed while this band reached $x = 62$ m at 10 m/s wind speed in the plain terrain.

Conspicuous differences of the concentration distribution on the x - y plane at an elevation of 2 m above ground in different terrains and wind speeds 5 minutes after the leakage starts are shown in Figure 12. The contour shows 5 m/s wind speed exhibited elevated risk of high concentration exposure. The highest concentration of the hazard zones developed after 5 min was 500 ppmv for a wind speed of 5 m/s and 200 ppmv for a wind speed of 10 m/s. The 200-ppmv hazard zone reached $x = 75$ m under 5 m/s wind speed in both plain and obstructed terrains. However, the 200-ppmv hazard zone for the 5 m/s wind speed appeared in wider shape near the front wall of the obstacle in the obstructed terrain. The 5-ppmv and 10-ppmv hazard zones for both wind speeds expanded laterally across the y range of 15–35 m in obstructed terrain while these hazard zone expanded across the y range of 19–31 m in plain terrain. Hence, the obstacle dispersed the gas in lateral direction.

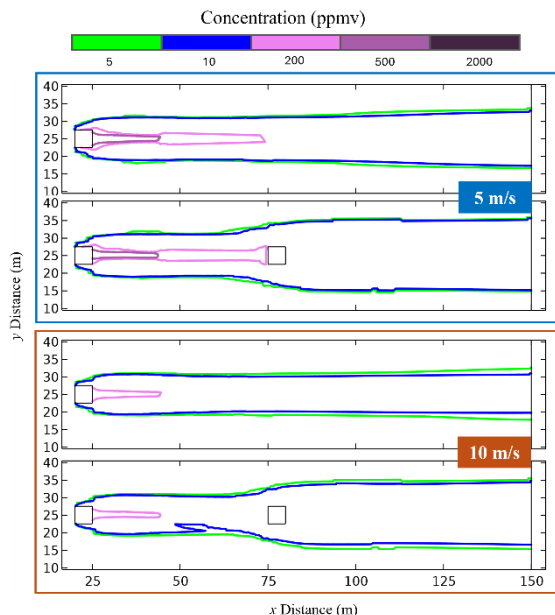


Figure 12. Concentration contour of 1,3-Butadiene after 5 min along x - y plane at $z = 2$ m for Case 1.

The effect of 5 m/s and 10 m/s wind speed on the gas dispersion in the Case 2 scenario is depicted in Figure 13. The enhanced horizontal transport of the species by a 10 m/s wind speed was observed.

Higher concentration zones were observed in the case of 5 m/s wind speed in the far field region compared to that for the 10 m/s wind speed. For instance, after 30 s, concentration of 1,3-butadiene at $x = 40$ m was in the range of 200–250 ppmv under 10 m/s wind speed while range of concentration at this distance was in the 400–500 ppmv range under 5 m/s wind speed. This observation reflects the stagnation phenomenon in a low wind speed and horizontal dispersion in a higher wind speed.

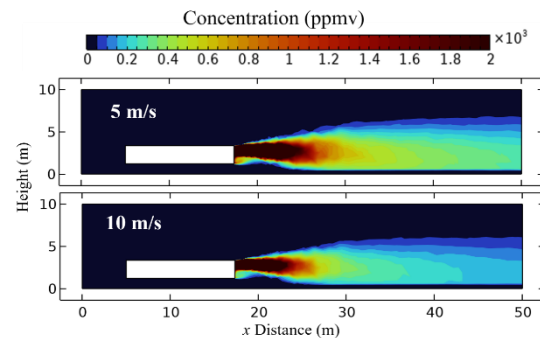


Figure 13. Concentration profile of 1,3-Butadiene after 30 s in 5 m/s and 10 m/s wind field for Case 2.

Similar to Case 1, riskier zones developed under 5 m/s wind speed at the elevation of 2 m above the ground as shown in Figure 14. The 200-ppmv hazard zone expanded beyond $x = 50$ m in 5 m/s wind speed while it reached $x = 45$ m in 10 m/s wind speed. The 500-ppmv hazard zone also occupied a larger area in 5 m/s wind speed compared to 10 m/s. Finally, the 2000-ppmv hazard zone which is immediately dangerous to life only appeared near the leaking point in the case of 5 m/s wind speed.

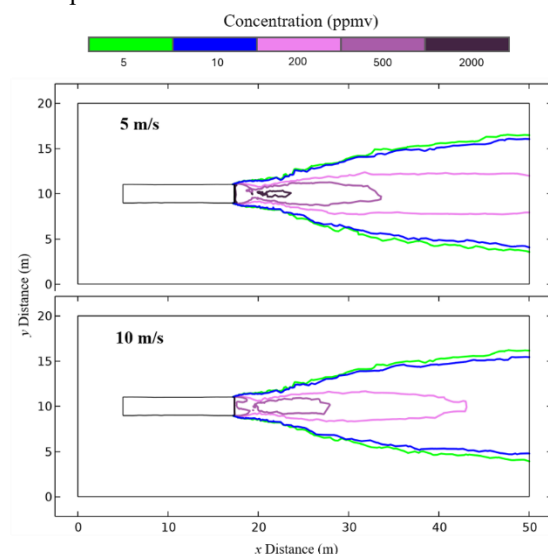


Figure 14. Concentration contour of 1,3-Butadiene after 5 min along x - y plane at $z = 2$ m for Case 2.

The gas release scenario of Case 2 was also simulated using EPA ALOHA to study the difference between integral model and CFD-based model. ALOHA estimates the cumulative footprint of the maximum hazard level reached at any time within a 1-hr window. In this ALOHA simulation a total 5 min 1,3-butadiene release was applied, and the model estimated the threat zone after 1 hour as presented in Figure 15.

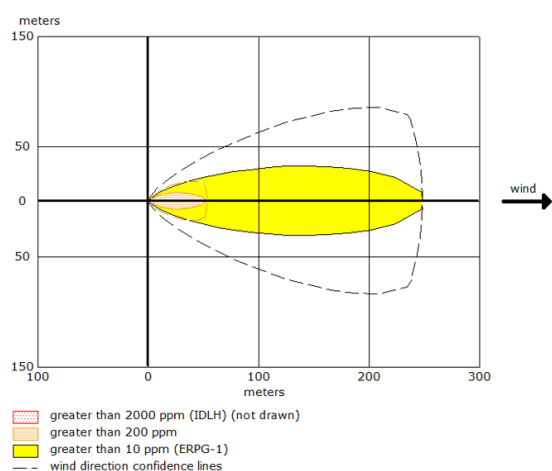


Figure 15. Threat zone estimated by ALOHA for 5 min 1,3-Butadiene release at 5 m/s wind speed.

The integral model like ALOHA provides cumulative footprint of the risk zone in 1 hour period. The CFD simulation can capture the transient variations of the concentration field immediately after the incident. Furthermore, local concentration accumulation can also be estimated by CFD simulation with the detailed calculation of the velocity field of wind altered by obstacles in the complex terrain.

Conclusions

The CFD-based model of toxic gas dispersion provided intuitive results of the concentration field varied by different terrain structures and wind speeds. The model could estimate concentrations of all points at any time throughout the exposure domain at local level. Higher wind speed facilitated the horizontal transport of the species but created a less acute hazard zone. On contrary, low wind speed exhibited stagnation effect on the dispersed gas, yielding to a high concentration zone across the domain. Obstacle showed blocking effect at the upstream gas flow field. Furthermore, obstructed terrain induces pronounced expansion of hazard zones in lateral direction compared to plain/flat terrain.

References

- (1) IARC Working Group on the Evaluation of Carcinogenic Risks to Humans. "1,3-Butadiene, Ethylene Oxide, and Vinyl Halides (Vinyl Fluoride, Vinyl Chloride, and Vinyl Bromide)", *International Agency for Research on Cancer*, Lyon, France Geneva, 2008.
- (2) B.E. Launder, and D.B. Spalding, "Two-Equation Models of Turbulence", *Lectures in Mathematical Models of Turbulence*, Academic Press: London/New York, pp. 90–110, 1972.
- (3) PubChem, https://pubchem.ncbi.nlm.nih.gov/compound/1_3-butadiene#section=Flash-Point. (accessed 2026-07-22).
- (4) D. A. Crowl, and J. F. Louvar, "Chapter 4. Source Models" *Chemical Process Safety*, 4th ed., Pearson, 2019.
- (5) Occupational Safety and Health Administration (OSHA), "1,3-Butadiene", 1996. <https://www.osha.gov/laws-regs/regulations/standardnumber/1910/1910.1051> (accessed 2026-07-01).
- (6) American Industrial Hygiene Association (AIHA). "ERPG/WEEL Handbook", 2016. https://downloads.regulations.gov/FAA-2019-0229-0021/attachment_1.pdf (accessed 2026-07-01).
- (7) Agency for Toxic Substances and Disease Registry (ATSDR). "Toxicological Profile for 1,3-Butadiene", 2012. <https://www.atsdr.cdc.gov/toxprofiles/tp28-c8.pdf> (accessed 2026-07-01).
- (8) National Institute for Occupational Safety and Health (NIOSH). "IDLH Value Profile for 1,3-Butadiene", 2017. <https://www.cdc.gov/niosh/docs/2017-107/> (accessed 2026-07-01).

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