Study of Impact of Terrain Structure on the Dispersion of Accidentally Released Air Pollutants

Sk. M. Manjur and S. Lin
Department of Chemical & Biomolecular Engineering, Lamar University, Beaumont, TX, USA.

Abstract

Toxic and hazardous air pollutants are released during chemical processes. Exposure to high concentration of toxic chemicals may cause serious health hazard and even death depending on the level of toxicity and severity of the chemical release condition. In the situation of an accidental release, emergency response and evacuation plan should be efficiently prepared to minimize the dire consequence. Additionally, chronic exposure to a hazardous chemical of a concentration higher than the permissible limit causes slow development of serious health problems. A mathematical simulation can provide comprehensive understanding about the dispersion trend of a chemical depending on its properties, ambient condition, and surrounding terrain structure. A proper planning for reduction of pollution along with efficient emergency response and rescue action plan can further be developed based on the understanding from mathematical simulation.

A finite element analysis model of a released toxic chemical from an industrial process unit into surrounding ambience has been developed using COMSOL Multiphysics 6.2. This high-resolution model executes precise and comprehensive calculations over small elements as the whole domain geometry is discretized into several small elements. Different scenarios in terms of terrain structure such as unobstructed, slightly obstructed, and complexly obstructed terrains are considered to study their impact on the chemical dispersion trend. The diffusion and convection of the released chemical through ambient air are the prevailing driving mechanisms of released chemical transport. The dispersion trend is estimated by the Fick's 2nd law of diffusion integrated with convection by velocity field of air. Different wind speeds and directions are applied to observe the effect of wind on chemical dispersion. Velocity field for the wind is established on the principle of compressible form of the Navier-Stokes and continuity equations. Transport and thermodynamic properties of air and chemical species are estimated at different temperatures and pressures. The calculated results are analyzed to study impacts of wind speed, ambient temperature and terrain type on the propagation of chemical species over time.

Keywords: Toxic Chemical Release, CFD, FEA

Introduction

Chemical process industries have a high risk of releasing toxic/ hazardous air pollutants during operation. Along with advancement of industrialization, this risk is increasing. Sudden exposure to high amount of toxic chemicals is dangerous to people near the facility including facility professionals and community residents. On the other hand, chronic low dose exposure to toxic chemicals has slow poisoning effects to human health. Entire environment is also affected by slow release or sudden accidental high amount release of toxic chemicals. Thus, both toxic chemicals release scenarios should be addressed and proper measures should be taken to protect the human life, environment and other resources from a catastrophic damage. Effective rescue plan and emergency evacuation plan can be established w a high-resolution dispersion trend of the released toxic chemical can be predicted. Computational model is a potential approach to predict the dispersion trend of released chemical. Dispersion trend depends on various factors such as: thermodynamic and physical properties of the chemical species, ambient conditions like temperature, humidity, wind speed & direction and structure of the exposure terrain.

Physical Model

In this study a chemical release model has been developed to simulate the dispersion trend of 1,3-Butadiene after sudden unplanned release. This work studied a dispersion from a storage tank (3 m × 3 m × 5 m) filled with pure 1,3- Butadiene at a pressure of 10 psig with a leakage from a 4 cm diameter hole located on the storage tank's wall. A 200 m × 200 m × 300 m region is considered as the exposure domain as shown in Figure 1.

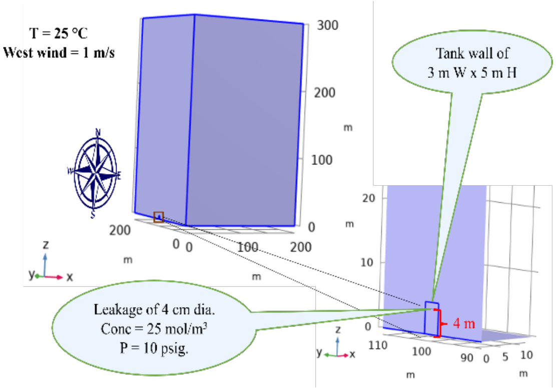

Figure 1. Sketch of the geometry used in this study.

The following is an example model when a west to east heading wind with a free stream velocity of 1 m/s flows into the domain and ambient temperature was set to 25 °C. Wind speed varies along the altitude height that is calculated numerically. Nominal height of atmospheric boundary is considered to be 274 m above ground. Wind speed changes within this layer until it reaches to a stable maximum value over this height.

1,3- Butadiene, one of the common toxic pollutants in petrochemical, plastic and rubber industries is selected as the released species. It is classified as carcinogenic by inhalation for human by US EPA. The toxicity level of 1,3- Butadiene in brief is listed in Table 1:

Table 1. The toxicity of 1,3- Butadiene.

Reference Concentration Level	0.001 ppm	Chronic exposure limit
OSHA PEL	1 ppm	Exposure up to 8 hr. a workday
AIHA ERPG-2 Level	200 ppm	Exposure up to 1 hr. in any incident
NIOSH IDLH	2000 ppm	Immediately dangerous to life

Two models have been developed in this study: one for plain terrain and another one for obstructed terrain with a building-like obstacle block of 5 m × 5 m × 10 m located at 20 m after the storage tank wall.

Reasonable mesh element size was chosen to balance the accuracy and computational time. Free tetrahedral and boundary layer meshing tools have been used to build the mesh. Maximum element size is 13.4 m and minimum element size is 4 m for the ambient air domain and smaller element sizes ranging from 7.4 – 0.8 cm was chosen for the zone around the leakage and tank wall. Five boundary layer mesh was built on the ground.

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.

Fluid Flow

The ambient air velocity field was calculated by Reynolds-average Navier Stokes equation. The *k-ε* Turbulent Flow interface was used for simulating single-phase flows at high Reynolds numbers. The flow was considered to be compressible. Reynolds-average Navier Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass were solved by the Turbulent Flow, *k-ε* interface.

The followings are the governing equations under this interface:

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}.\nabla)\boldsymbol{u} = \nabla\cdot[-pI + (\mu + \mu_T)(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T)] + F \tag{1}$$

$$\rho\nabla\cdot(\boldsymbol{u}) = 0 \tag{2}$$

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

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

$$\mu_T = \rho C_\mu\frac{k^2}{\epsilon} \tag{5}$$

$$P_k = \mu_T[\nabla\boldsymbol{u}:(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T)] \tag{6}$$

Physical and thermodynamic properties of air are calculated based on the ambient conditions specified for the model.

Wind speed changes along the height altitude. The elevation along which the wind speed is affected by topography is the atmospheric boundary layer. The wind speed profile within this layer is given by:

$$V_z = V_g\left(\frac{Z}{Z_g}\right)^{\frac{1}{\alpha}} \tag{7}$$

where,

V_Z = mean wind speed at height Z above ground

V_g = Gradient wind speed assumed constant above the boundary layer

Z = Height

Z_g = Nominal height of boundary layer

α = Power law coefficient

Mass Transport

To calculate the mass transport of chemical species by diffusion and convection, Transport of Diluted Species physics was used. Diffusion coefficient, density, dynamic viscosity of 1,3- Butadiene were used as physical and transport properties of the species. The Fick's 2nd law of diffusion is the basic principle of this calculation. The governing equations are:

$$\frac{\partial c_i}{\partial t} + \nabla.(-D_i\nabla c_i) + \mathrm{u}\cdot\nabla c_i = R_i \tag{8}$$

$$N_i = -D_i\nabla c_i + \mathrm{u}\cdot\nabla c_i \tag{9}$$

where,
c_i = Concentration of the species
N_i = Mass flux
D_i = Diffusion coefficient of the species

Initial & Boundary Condition

Initial condition was set as no leakage and no 1,3-Butadiene in the ambient air. The leakage started 30s after the computation started.

Boundary conditions of the Fluid Flow physics were deployed as the followings. Wind flows from west to east; west face of the domain was set as inlet air with varying speed along the height. The ground, tank wall and obstacle walls were set as no slip condition. East, north, south and top face is set as outlet with a pressure of 1 atm. Pressure at the leakage is set to be10 psig.

Boundary conditions of the Mass Transport physics was chosen as the concentration in the leakage is 25 mol/m^3.

Simulation Results

Concentration profile of the species was observed with time and different spatial distance. The dispersion trend is noticeably different in different terrain type. Figure 2 shows the concentration profile and history of released 1,3- Butadiene. The range of the concentration color table has been set as 0 – 2,000 ppm to show the high-risk zone according to critical concentration level of 1,3-Butadiene.

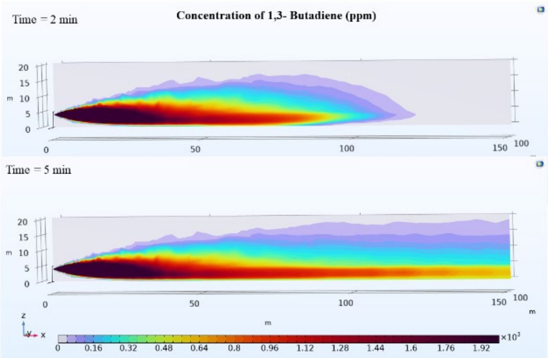

Figure 2. Concentration profile of 1,3- Butadiene along x-axis after 2 min & 5 min in plain terrain.

The concentration of 1,3- Butadiene buildup around the obstacle is significantly higher as shown in Figure 3. Concentration did not reach up to 2,000 ppm at the distance x = 150 m in the obstructed terrain while it reached 2,000 ppm at this distance in case of plain terrain. Rather, the species accumulates with notable amount around the obstacle. Concentration is tremendously higher at the front and back zones of the obstacle.

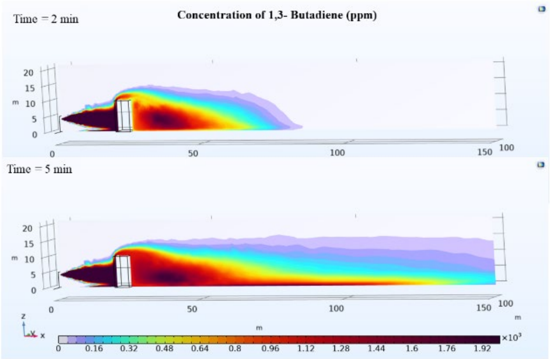

Figure 3. Concentration profile of 1,3- Butadiene along x-axis after 2 min & 5 min in obstructed terrain.

Figure 4 shows how far and wide the 1,3-Butadiene transports at 1.5m above the ground (average human eye level) when the leakage is located at 4 m above the ground. Concentration profile after 2 min. and 5 min are presented for both types of terrain.

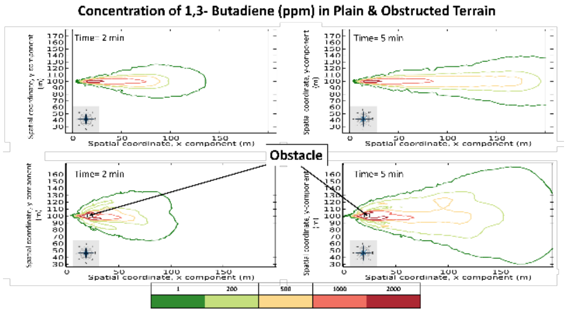

Figure 4. Top View of Spatial Dispersion of 1,3-Butadiene at 1.5 m Above ground.

Terrain type influences how long and wide distance will be covered by 1,3- Butadiene. 1,3- Butadiene travels long distance from the source in plain terrain while it spreads through wider area in the terrain with obstacle, which is depicted in Figure 5.

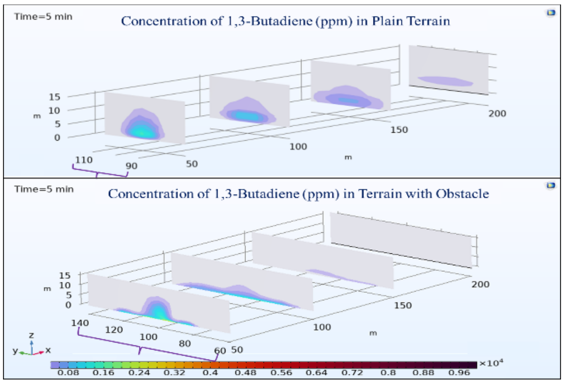

Figure 5. Spatial Dispersion of 1,3- Butadiene after 5 min.

Concentration buildup around the obstacle is shown in Figure 6. Concentration near the front face of the obstacle increases above 10,000 ppm very soon after the release incident. Around the back face of the obstacle, 1,3- Butadiene starts to concentrate and keep increasing over time.

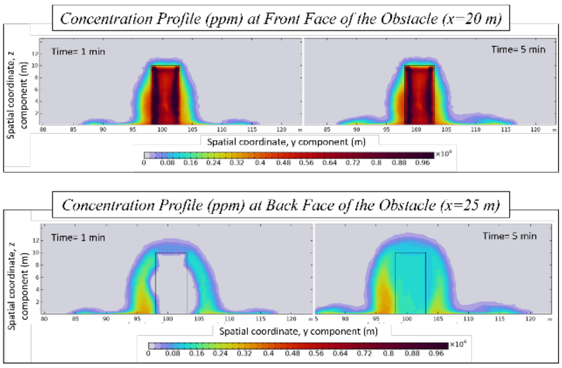

Figure 6. Concentration Profile at Front Face of the Obstacle.

Conclusions

This study provides a comprehensive idea about the dispersion behavior of 1,3- Butadiene depending on the terrain type. It is observed that, the gas concentration gets higher around obstacles such as building, process unit or other kind of infrastructure. The chemical accumulation occurs around the wall specially the hindering wall such as front wall of the obstacle because wind flow is hindered by that wall. The species gets enough room to blow away in a plain terrain and reaches to longer distance from the source compared to the obstructed one. On the other hand, it spreads in wider area in the obstructed terrain compared to the plain one.

Dispersion trend varied greatly with wind speed and direction. Further study will be carried out to examine the effect of wind speed and direction, different temperature and humidity level. Released chemical's dispersion on more complex terrain will be studied in future. Predicted ambient conditions due to climate change will be integrated in future work to study the effects of climate change on the accidental release scenario.

References

[1] H. Zhu & J. Jing, "Numerical Simulation of Gas Leaking Diffusion from Storage Tank", *Communications in Computer and Information* Science, vol. ICICIS 2011, pp. 416 – 421, 2011.

[2] A. Fiorucci *et al,* "Risk Assessment of Dangerous Products Release and Dispersion: a Comparison Between CFD and Integral Models", *Chemical Engineering Transactions,* vol.13, pp.195–200, 2008.

[3] Y. Gan & Y. Wang, "A Case Study on Optimization of Urban Design Base on Wind Environment Simulation", *Journal of Civil Engineering and Architecture,* vol.10, pp.870-880, 2016.

[4] Occupational Safety and Health Administration (OSHA). Occupational Safety and Health Standards, Toxic and Hazardous Substances. Code of Federal Regulations. 29 CFR 1910.1000. 1998.

[5] American Industrial Hygiene Association (AIHA). The AIHA 1998 Emergency Response Planning Guidelines and Workplace Environmental Exposure Level Guides Handbook. 1998.

[6] National Institute for Occupational Safety and Health (NIOSH). Pocket Guide to Chemical Hazards. U.S. Department of Health and Human Services, Public Health Service, Centers for Disease Control and Prevention. Cincinnati, OH. 1997.

Acknowledgements

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Biological and Environmental Research Program under Award Number DE-SC0023216.
We would like to thank Dr. Xianchang Li, Professor, Department of Mechanical Engineering, Lamar University for his advice on CFD regarding calculation of velocity field of ambient wind.