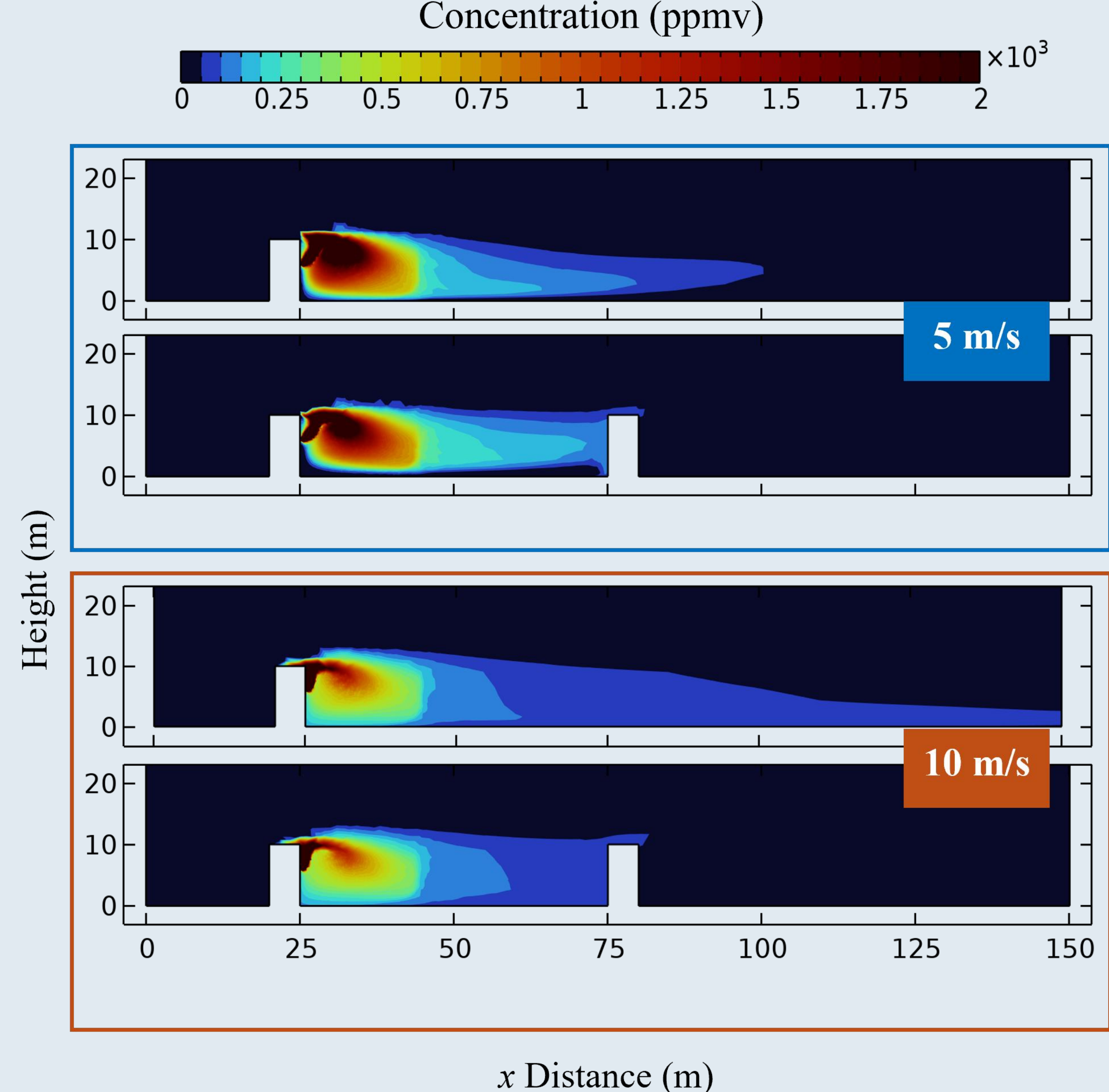




Introduction

More than 1,000 of the 102,177 hazardous chemical incidents during 2021–2024 were HAZMAT releases posed public health threats, with Texas leading in such releases, followed by California, Ohio, and Louisiana. Proper prediction of the dispersion trend of the released chemical is essential to construct efficient emergency response plan within short time after the accident to safeguard the people, properties and the environment.

CFD simulation was used to study the dispersion of released chemicals from different storage tanks in the air. Released species' concentration accumulation and dilution in spatial and temporal scale were captured by a 3D CFD simulation through detailed estimation of velocity field across the exposure domain.

Methodology

A hypothetical scenario of a leakage from a partially filled liquid main storage tank of 1,3-Butadiene was simulated using Ficks 2nd law coupled with CFD. The $k-\epsilon$ turbulence model was used to calculate the velocity fields of wind and released gas. The discharge flowrate and velocity of released gas were calculated using the following equations assuming a constant tank pressure (P_v) resulting from vapor liquid equilibrium.

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

$$u_l = \sqrt{\frac{2 g_c C_0^2 R T_0}{M} \times \frac{\gamma}{\gamma - 1} \times \left[1 - \left(\frac{P_{down}}{P_1} \right)^{\frac{\gamma-1}{\gamma}} \right]}$$

FIGURE 1. Chemical storage condition and pressure inside the tank (Left). Boundary conditions in different geometries with main storage tank (Middle) and intermediate horizontal bullet storage tank (Right).

A constant leak speed of 50 m/s was assumed in a case of a horizontal bullet shaped intermediate 12,000 US gallon storage tank.

Results

Integral model like ALOHA estimates the cumulative footprint of the maximum hazard level reached at any time within a 1-hr window. CFD model offers transient concentration profile from the beginning of the release. It can capture micrometeorological phenomena such as recirculation and vortex formation around the surfaces and obstacles across the exposure domain. Therefore, concentration of the released species affected by the velocity field of wind can be properly estimated by CFD-based simulation. Exposure risk severity demonstrates inverse wind speed dependency, reflecting the interplay between atmospheric dilution capacity and pollutant concentration dynamics.

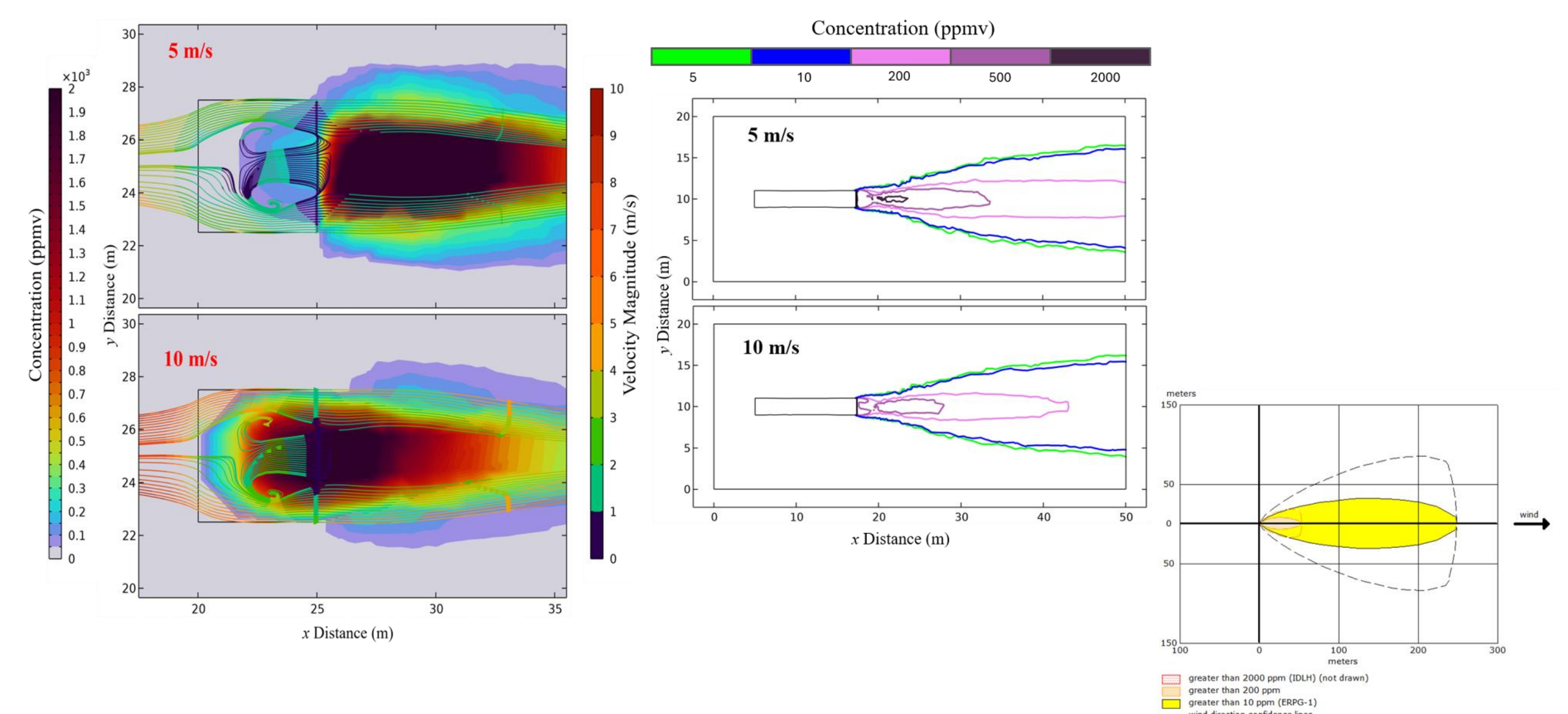


FIGURE 2. Concentration profile of 1,3-Butadiene and velocity streamline over the roof of storage tank in plain terrain after 5 min of release from a 66,000 US gallon main storage tank (Left); 12,000 US gallon intermediate bullet storage tank (Middle) under 5 m/s and 10 m/s wind speed; 1-hr threat zone estimated in ALOHA simulation for 5 min release of 1,3-Butadiene from an intermediate bullet tank (Right).

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