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EXTENDED ABSTRACT

Abstract title : Simulation of Accidental CO_2 Releases in Urban Areas

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Abstract

This article explores the simulation of pressurized CO_2 release at the “Centre d’Entraînement aux Actions en Zone Urbaine” (CENZUB), a large-scale training site in Sissonne, northeastern France, using two distinct modeling approaches. The first involves passive scalar emission, while the second simulates a pressurized jet through mass injection under the assumption of compressible flow. Both methods are compared against experimental data to evaluate their accuracy and applicability. While the passive scalar method tends to overestimate dispersion near the source, it benefits from compatibility with precomputed steady wind fields, significantly reducing computational cost. In contrast, mass injection better captures the interaction between the jet and the surrounding flow, making it better suited for such scenarios. Thus, the compressible Eulerian simulation provides a robust framework for accurately modeling turbulent dispersion near the source.

Introduction

Atmospheric dispersion of gas releases presents a significant challenge in both environmental engineering and fluid mechanics. Accurate understanding and modeling of these processes are crucial for evaluating environmental and public health risks, especially in urban settings where complex infrastructure profoundly influences flow dynamics. Within this context, numerous experimental studies have been conducted over the past decades (e.g., [1], [2]), often employing arrays of regular obstacles to simulate idealized urban environments. These setups provide valuable insights into dispersion mechanisms and serve as benchmarks for validating numerical models.

To assess the influence of complex environments on gas dispersion, INERIS recently conducted a controlled pressurized CO_2 release experiment as part of a broader initiative aimed at integrating industrial risk assessment into urban safety training [3]. The campaign generated high-resolution experimental data, including gas concentration at multiple locations. Accidental releases related to pressurized CO_2 pipelines above the ground yield to a high velocity jet, and a temperature drop [4] that may pose challenges when reproducing it at a local scale. This study compares the performance of two modeling approaches for simulating such pressurized heavy gas releases. Reynolds-Averaged Navier–Stokes (RANS) simulations are carried out using code_saturne [5], employing a compressible flow scheme [6]. The first approach involves passive CO_2

injection, while the second uses mass injection to simulate the jet dynamics. A passive CO_2 injection is considered first, followed by a mass injection. Local numerical CO_2 concentration is compared to the measurements to access both simulations accuracy. After describing the experimental campaign, the numerical settings are presented, followed by the validation results.

Experimental campaign description

The experiments conducted by INERIS [3] involved the release of pressurized CO_2 directed toward a high-rise building within the urban test zone (see Figure 1, left). The setup was specifically designed to replicate the interaction of a dense gas jet with complex urban geometries, with a focus on flow behaviour and pollutant dispersion around built structures. This paper concentrates on the first experiment from the reference study, which involved a mass flow injection of 7 kg/s sustained over 127 seconds. CO_2 was released through a 2-inch diameter pipe connected directly to a truck, where the gas was stored under saturation conditions at 15 bars. Gas concentration measurements were obtained using multiple technologies—including infrared sensors, catharometers, and thermal conductivity detectors (Tk)—to ensure consistency and reliability of the data. Additionally, two weather stations positioned upstream and downstream of the release site recorded wind speed and direction, temperature, and humidity, providing essential boundary conditions for numerical modeling.

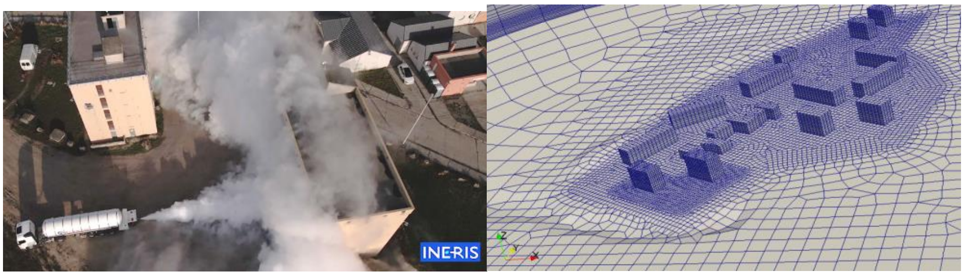

Figure 1: (left) Impinging release against a high-rise building [3]. (right) Numerical mesh used.

Numerical setup

Numerical simulations were performed using a computational domain designed to replicate the urban layout of the CENZUB site (Figure 1, right). A structured mesh comprising 274,084 cells was generated, with local refinement applied near the release point and building surfaces to accurately resolve flow gradients and turbulent structures. Boundary conditions included a logarithmic wind profile at the inlet, a pressure outlet at the domain exit, and no-slip conditions on all solid surfaces. The simulations employed a Reynolds-Averaged Navier–Stokes (RANS) solver with a linearized k–ε turbulence model. Time-dependent simulations were conducted using a variable time step to capture transient plume dynamics while maintaining numerical stability. The atmospheric module of code_saturne is used with a compressible time scheme and a second order spatial scheme.

The CO_2 injection conditions were determined based on the assumption of adiabatic expansion within the release pipe. This thermodynamic hypothesis enables the estimation of the jet's exit velocity and temperature, which are incorporated into the simulation as momentum and energy source terms, in addition to mass and gas mass fraction inputs. Under these conditions, CO_2 exits the pipe at an estimated temperature of 130.16 K (–143.15 °C) and a velocity of approximately 849.6 m/s. These values reflect the rapid decompression of the pressurized gas and are critical for accurately capturing the jet's initial momentum and thermal characteristics. Due to mesh resolution constraints—specifically, the injection diameter being smaller than the mesh cell size—the source terms are applied over a larger computational cell. This approximation introduces some limitations but remains necessary to ensure numerical stability and consistency within the simulation framework. Two simulation strategies are tested in this study. The first, referred to as EPI (Eulerian Passive Incompressible), models passive gas injection without affecting mixture density and dynamics. The second, called EAC (Eulerian Active Compressible), includes mass, energy, and momentum injection, and accounts for density variations using Dalton's law for ideal gas mixtures. Due to differing wind directions recorded at the two weather stations (~125° and ~325°), a wind direction of 225° was used.

Results and Discussion

Qualitative and quantitative comparisons are made between EPI and EAC simulations. Figure 2 shows a horizontal slice of CO_2 concentration at the injection height, 125 seconds after release with a 270° wind angle. The plume dispersion differs significantly between the two approaches: EAC captures jet dynamics and impingement effects, while EPI neglects these, resulting in unrealistic near-field accumulation due to the absence of buoyancy and momentum considerations.

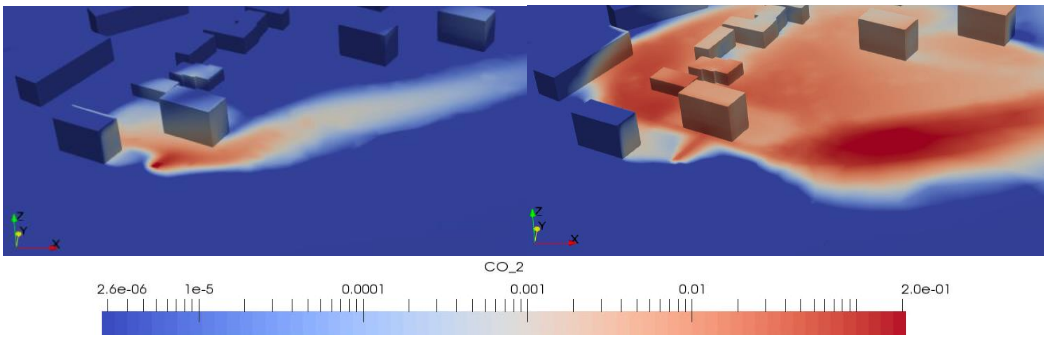

Figure 2: Slice of the CO_2 mass fraction after 125 s of injection using a wind direction of 225°. (left) EPI. (right) EAC. Scale was set for visualisation purposes.

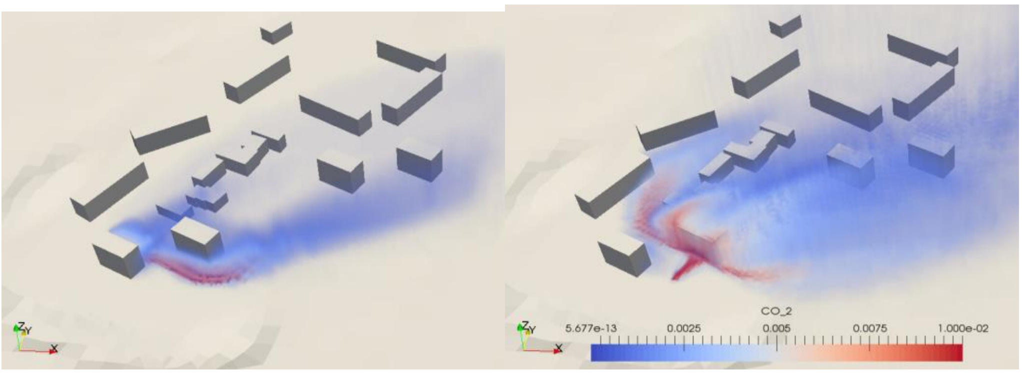

Figure 3. Gas dispersion plume after 125 s of injection. (left) EPI. (right) EAC. Scale was set for visualisation purposes.

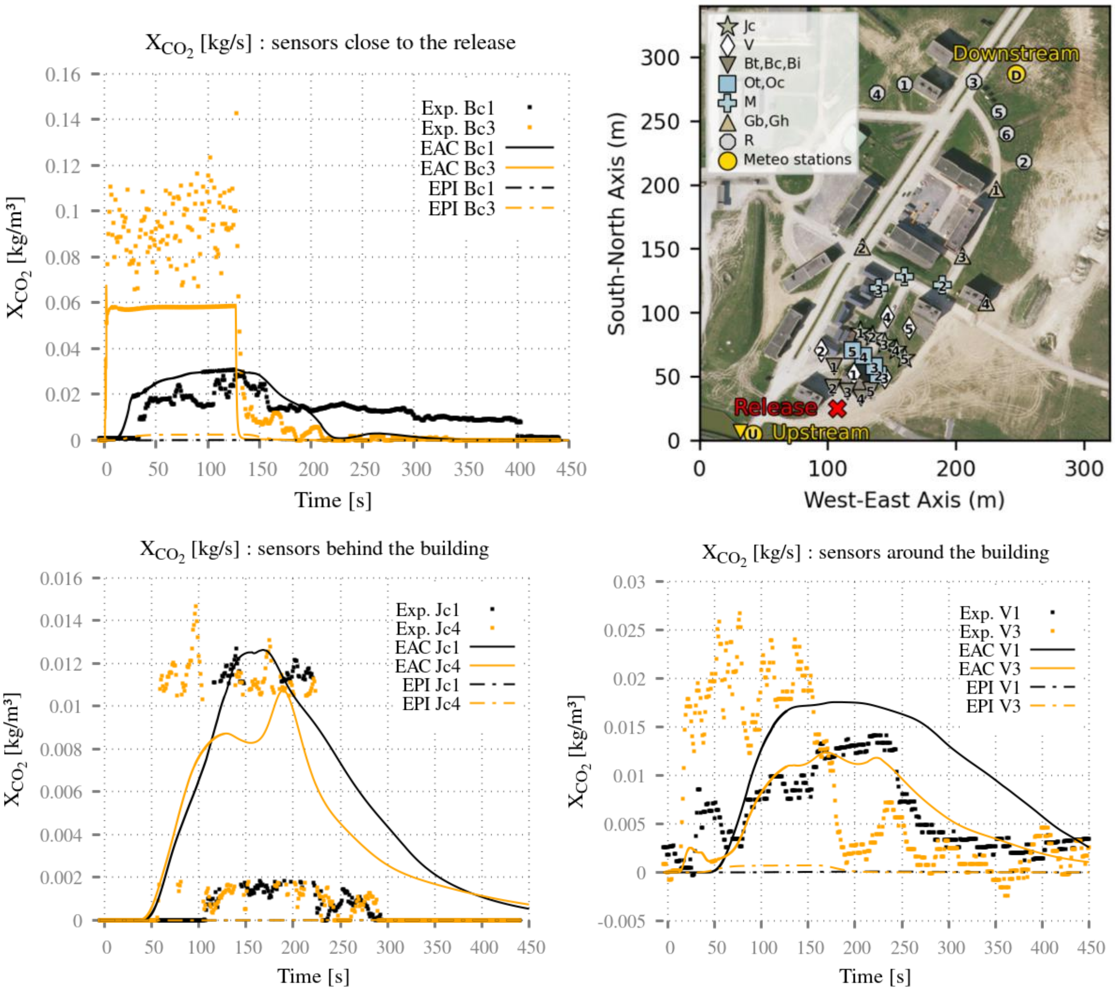

Figure 4. CO_2 concentration over time for different sensors located close to the release (top left), behind the impacted building (bottom left), and round the building (bottom right). Sensor's location for the simulated experiment, from [3].

Figure 3 presents the CO_2 plume from both EPI and EAC simulations. While the scalar is transported by the wind for the EPI simulation, the jet impinges on the building, lifting the gas cloud, which is then advected by the wind for the other. The resulting plume shape closely resembles the photo in Figure 1 (left), although the image is not time-synchronized with the release. Quantitative results are shown in Figure 4, illustrating CO_2 mass concentration sensors located in the jet zone (sensor positions indicated in Figure 4, top-right). The EPI simulation fails to reproduce the observed dispersion, with no detectable concentration at the sensors. In contrast, the EAC simulation, which accounts for jet dynamics, provides a more accurate prediction, with concentrations near the expected average. The EPI results are expected, as the plume follows the wind direction.

Conclusion

This study represents an initial step in validating the atmospheric module of code_saturne for simulating pressurized heavy gas releases in urban environments. The complex geometry of the CENZUB site was incorporated into the computational mesh, and two simulation approaches were tested—passive (EPI) and active (EAC) source term injection. Results indicate that passive scalar transport fails to reproduce the observed plume dynamics, particularly near the source. In contrast, the active injection approach, which captures jet impingement and buoyancy effects, yields more realistic dispersion patterns. However, sensitivity to wind direction remains a key challenge. Future work will focus on refining the mesh near the jet zone, better representing wind variability, and exploring alternative modeling strategies such as the stochastic Lagrangian approach [7, 8].

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References

[1] Biltoft, C.A. Customer Report for Mock Urban Setting Test; DPG Document 8-CO (2001): 160-000; Defense Threat Reduction Agency: Alexandria, VA, USA, 2001.

[2] Fox, S.; Hanna, S.; Mazzola, T.; Spicer, T.; Chang, J.; Gant, S. Overview of the Jack Rabbit II (JR II) field experiments and summary of the methods used in the dispersion model comparisons. Atmos. Environ. 2022, 269, 118783.

[3] Joubert, Lauris, et al. "Experimental Campaign of Massive CO2 Atmospheric Releases in an Urban Area." *Atmosphere* 14.9 (2023): 1428.

[4] Pham, L. H. H. P., & Rusli, R. (2016). A review of experimental and modelling methods for accidental release behaviour of high-pressurised CO2 pipelines at atmospheric environment. *Process Safety and Environmental Protection*, *104*, 48-84.

[5] EDF R&D. Code_saturne. *https://www.code-saturne.org/cms/web/*.

[6] Amino, Hector, et al. "A time-staggered second order conservative time scheme for variable density flow." *International Journal for Numerical Methods in Fluids* 94.12 (2022): 1964-1995.

[7] Minier, Jean-Pierre, Martin Ferrand, and Christophe Henry. *Understanding Turbulent Systems: Progress in Particle Dynamics Modeling*. Springer Nature, 2025.

[8] Balvet, Guilhem. *Lagrangian Modelling of gas/particle pollutant dispersion for atmospheric flows within stable, neutral and unstable situations*. Diss. École des Ponts ParisTech, 2024.