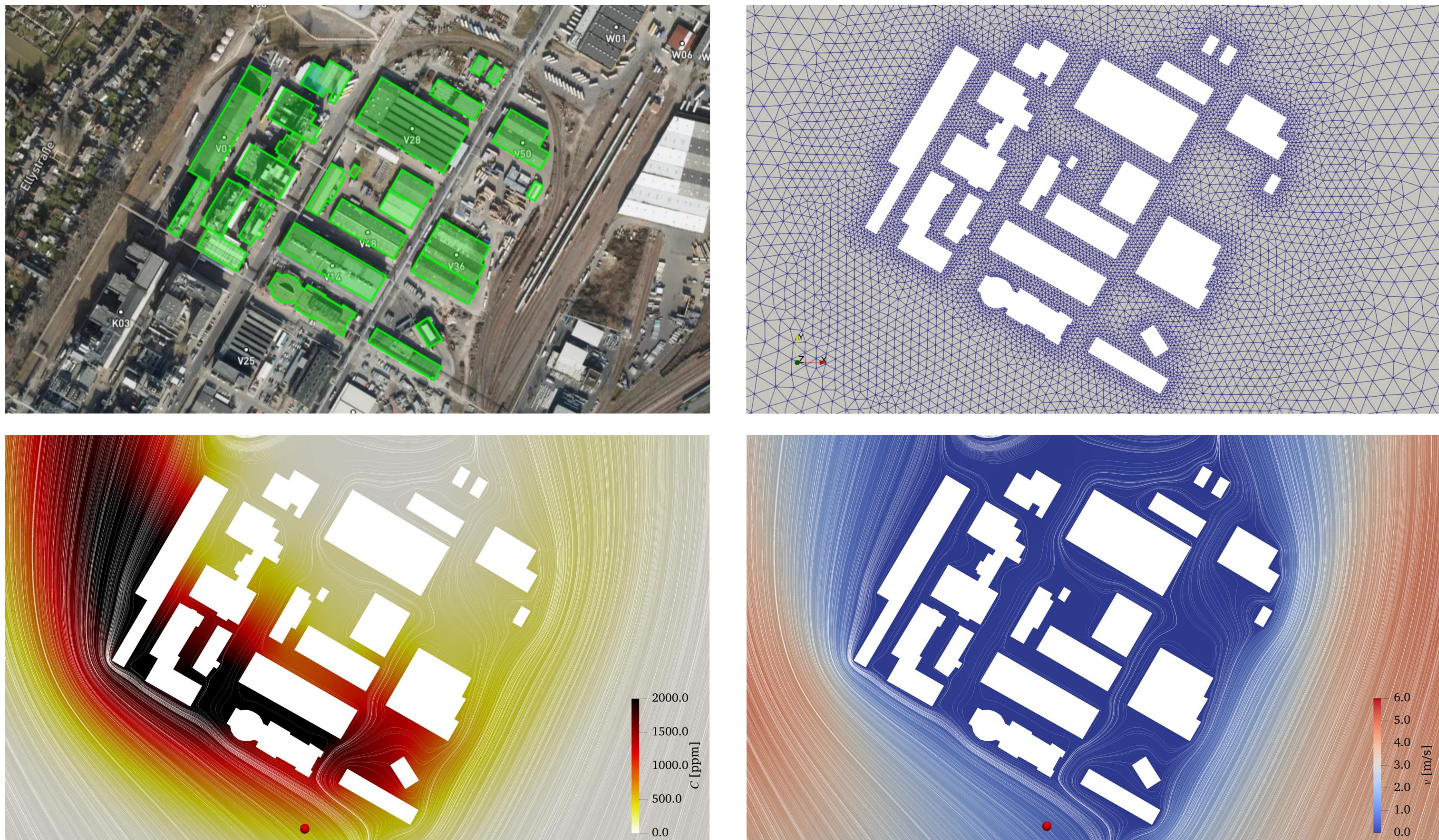


# CONTAMINANT DISPERSION SIMULATION IN A DIGITAL TWIN FRAMEWORK

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Top-left to bottom-left, clockwise: topography acquisition via georeferenced databases, analysis domain reconstruction, wind field, contaminant concentration. ©Mapbox, ©Openstreetmap, ©Maxar.

## Motivation

During emergencies, timely predictions of airborne contaminant dispersion are imperative to assess the level of threat to civil security and to establish an informed **real-time decision-making** process. This is essential to effectively evacuate civilians and guarantee the functionality of critical infrastructures.

## Computational framework

The prediction is based on a simulation process structured in three parts:

- Generation of desired geometry;
- Evaluation of wind flow field;
- Calculation of contaminant concentration evolution.

In the first preparatory step, the computational domain required for the solution of the dispersion problem is automatically generated through a query to a **geo-referenced database**. Here, the landscape geometrical features necessary for an accurate evaluation of the wind velocity field

are collected through specific semantics, and employed for the automatic generation of a **finite element mesh**. In a following stage, the incompressible **Navier-Stokes equations** are solved numerically on this domain, based on specific boundary conditions accounting for desired wind directions and intensity. In a third and final step, the evaluated wind field is used as a background vector field in the definition of a **transient advection-diffusion problem** whose solution provides the evolution of an airborne contaminant concentration in space and time. Different scenarios can be taken into account in this model, including, but not limited to, an initial dispersion confined in time or a continuous and persistent leakage. The wrapping in a Bayesian multi-fidelity analysis framework allows for **considering uncertainties** in the model inputs.

## Digital twinning

The computational paradigm is easy to extend by additional features that make it appealing for a synergetic integration in a **digital twin (DT)** framework.

Even though no unique definition exists, a DT can be described in a general sense as: **“A live digital coupling of the state of a physical asset or process to a virtual representation with a functional output”** [1] and its development opens new possibilities in the context of critical infrastructure protection (CIP).

Concerning this specific application, a two-way coupling can be implemented by gathering **real-time sensor data as input** for the solution of the two sets of equations in steps (ii) and (iii), while the model output is meant to be employed in an **informed decision making** process with a human in the loop. Since real-time data exchange is fundamental, the most computationally heavy steps (i) and (ii) can be performed offline and the related results updated only when necessary.

## Further developments

In the future, the framework will be enhanced by two additional features. Firstly, a faster assessment of the wind field can be achieved applying intrusive and non-intrusive **reduced order models** to boost computational efficiency while maintaining accuracy; secondly, leveraging on the acquired data, the model can assist **optimal sensor placement** strategies.

The project defines an automated workflow to simulate air contaminant dispersion in built environments. The goal is the creation of a reliable predictive model of a hybrid digital twin to provide informed real-time assistance in the context of evacuation scenarios.

[1] H. Boyes and T. Watson, “Digital twins: An analysis framework and open issues”, *Computers in Industry*, vol. 143, p. 103763, 2022.