

# Large Scale Outdoor Flammable & Toxic Gas Dispersion Modelling in Industrial Environments

## Introduction

The prediction of an accidental gas release, whether toxic or flammable, in terms of people, assets and production is vitally important in terms of reducing the impact from such a Major Accidental Hazard (MAH).

When conducting consequence analysis of gas releases, integral models are widely used.

Geometrically complex scenarios (e.g. buildings, structures, process units, towers etc) and non-flat terrain (e.g. hills, inclines, descents etc) make integral models inaccurate and require more rigorous calculation Methods, such as Computational Fluid Dynamic (CFD) simulations, in order to obtain more accurate estimates of the dispersed cloud extent and its effect.

## Model Description & Validations

HazRes' CFD Gas Dispersion Model, using COMSOL, is a three-dimensional (3D) model adapted to simulate atmospheric airflow and dispersion simulation.

The model and solver provide simulations based on the Eulerian approach, utilizing an un-structured grid, finite element method to model atmospheric air flow and dispersion at full scale and fine resolution. It also has the ability to model the interaction with complex terrain and obstacles using the k-epsilon turbulence closure model.

HazRes' Model has been validated against both experimental results as well as an industry standard integral model for which it is in good agreement.

## Discussion & Conclusions

It is believed that the results presented demonstrate the capability of HazRes' CFD Gas Dispersion model, solved using COMSOL Multi-Physics, and its capability to perform both stationary and transient time-dependent analyses of flammable and toxic gas releases over large geographic areas, complex terrains and structures.

## Case 1: Exhaust Stacks near a Hill

HazRes has used its CFD Gas Dispersion model in COMSOL to model a Carbon Dioxide (CO<sub>2</sub>) rich exhaust plume from three (3) different height and diameter exhaust stacks at the base of a hypothetical hill. The three (3) exhaust stacks measure 25m, 50m and 100m in height.

The computational volume has a footprint of 2km by 2km and the wind profile was logarithmic with height in a direction prevalent to the inclination of the hill. HazRes conducted a transient time-dependent analysis on the exhaust gas release in order to determine the cloud spread, extent and possible touchdown (cloud touches the ground) as a function of time.

The time-dependent results are shown in **Figure 1** of iso-concentration plots from the three (3) exhaust stack gas cloud dispersions.

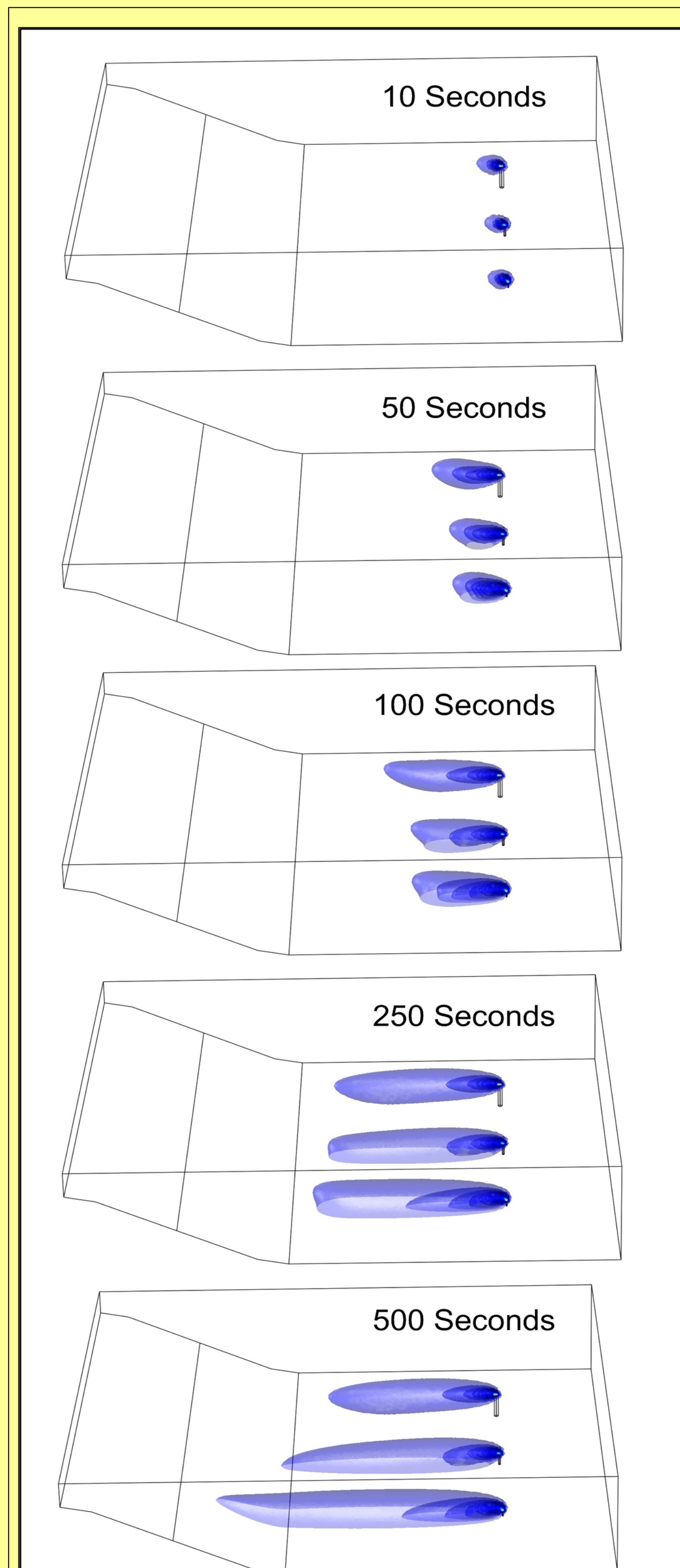


Figure 1. Iso-Concentration Plots showing Exhaust Stack Gas Dispersion with Time including Cloud Touchdown.

## Case 2: Onshore CH<sub>4</sub> Release

HazRes has modelled a methane (CH<sub>4</sub>) release in a hypothetical industrial onshore facility, using its CFD Gas Dispersion Model in COMSOL as shown in **Figure 2**.

The aim of this particular exercise is to demonstrate how the model can be used to locate fixed stationary gas detection sensors at a facility. The source of the release is a 10m high vessel. The computational volume has a footprint of 400m by 400m and the wind profile is logarithmic with height set at an angle of 30° from the X-axis anti-clockwise. In total, six (6) fixed gas detection sensors were located both upstream and downstream of the point of release as shown in **Figure 3**.

In this particular example, the issue of concern is the concentration of methane in air that could provoke an explosion, if ignited. Therefore HazRes is interested in both the Lower Explosive Limit percentage for methane in air (LEL%) which is 5% (i.e. 50,000ppm) and 50% LEL which is 2.5% (i.e. 25,000ppm), purely as a safety factor.

**Figure 4** shows the predicted methane concentration levels as a function of time for each of the six (6) fixed gas detector sensors.

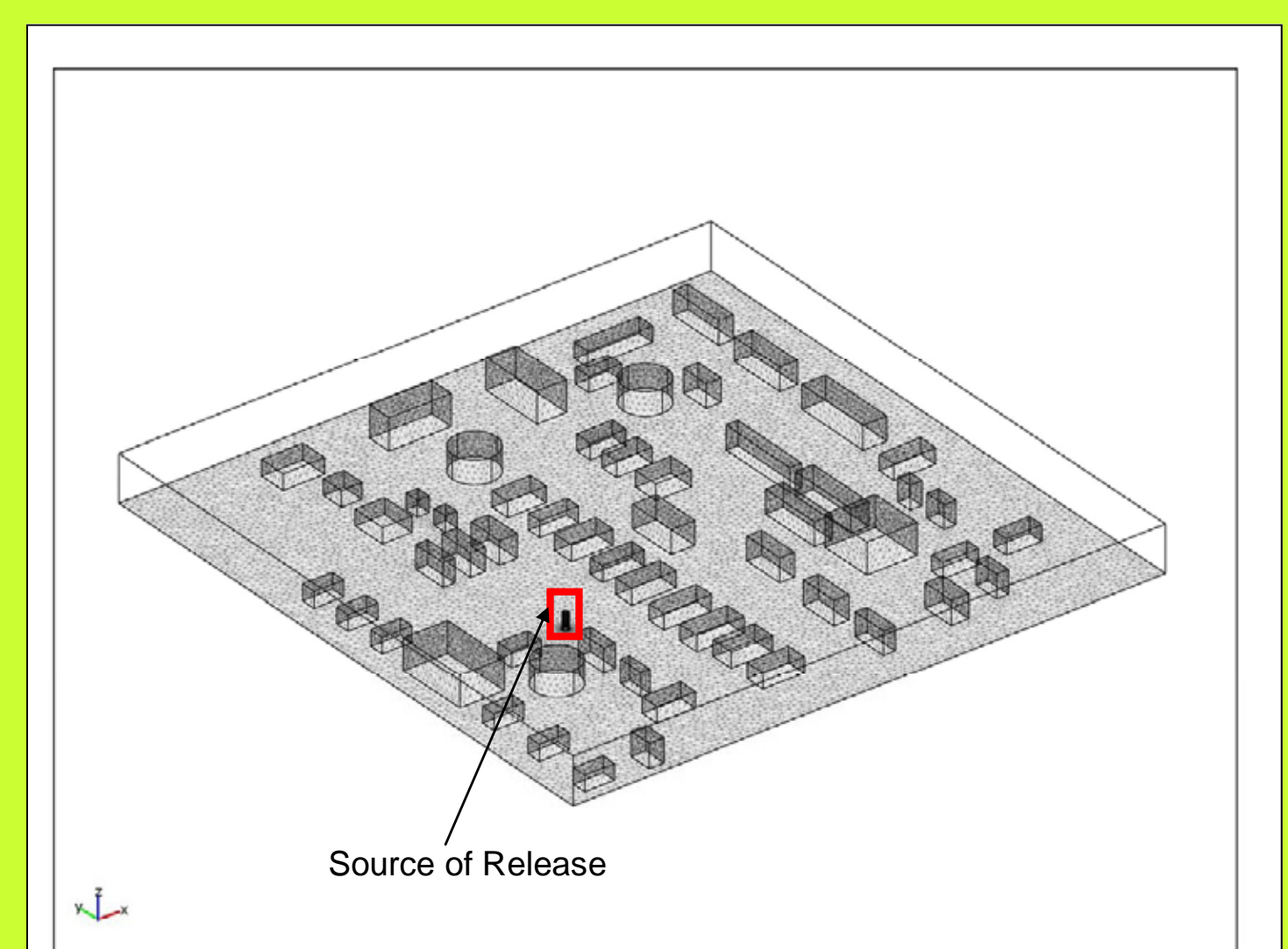


Figure 2. Computation Volume Model in COMSOL of Industrial Site and Source of Release

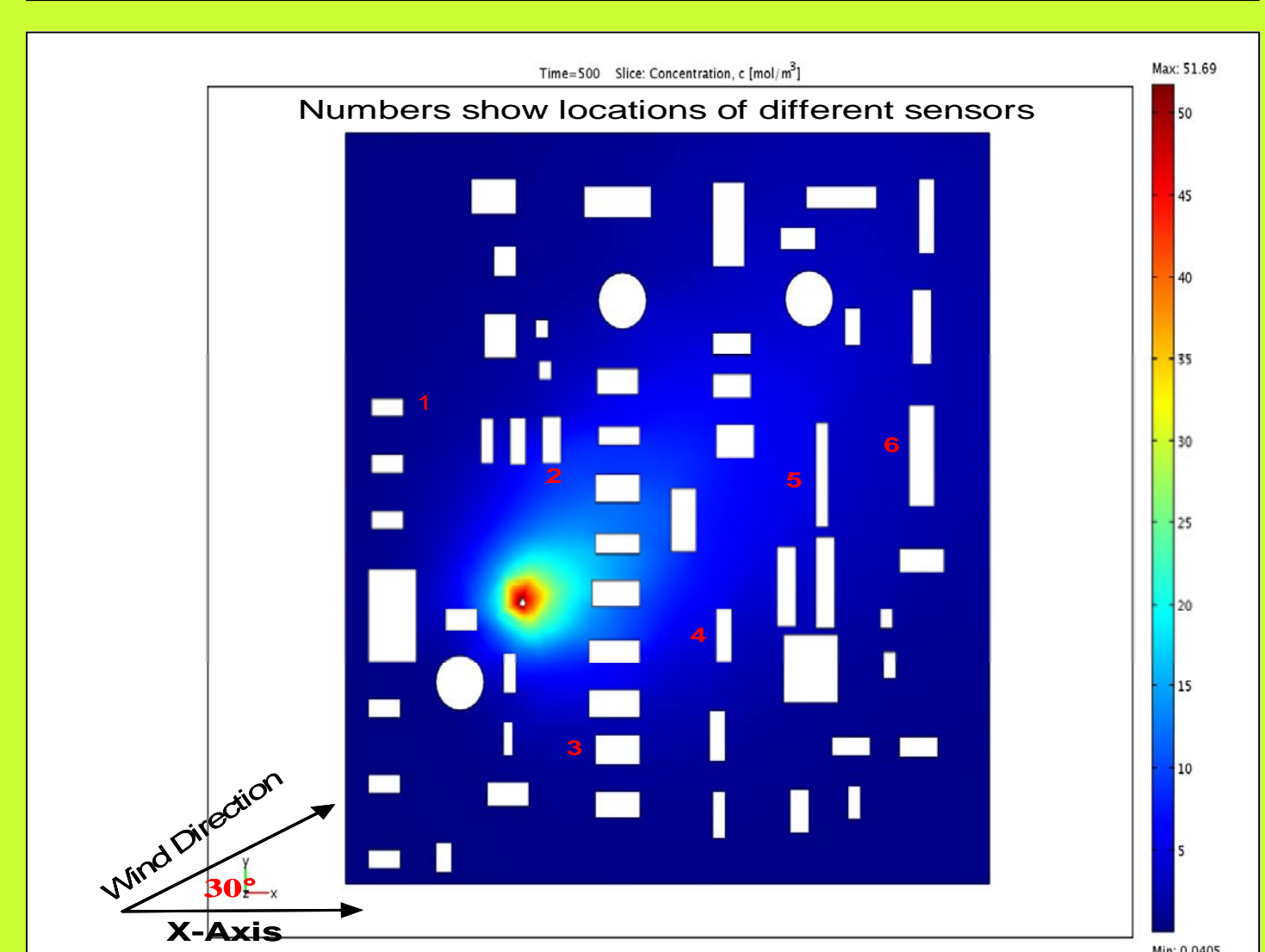


Figure 3. Plan View of Onshore Facility showing Locations of the Six Fixed Gas Detector Sensors.

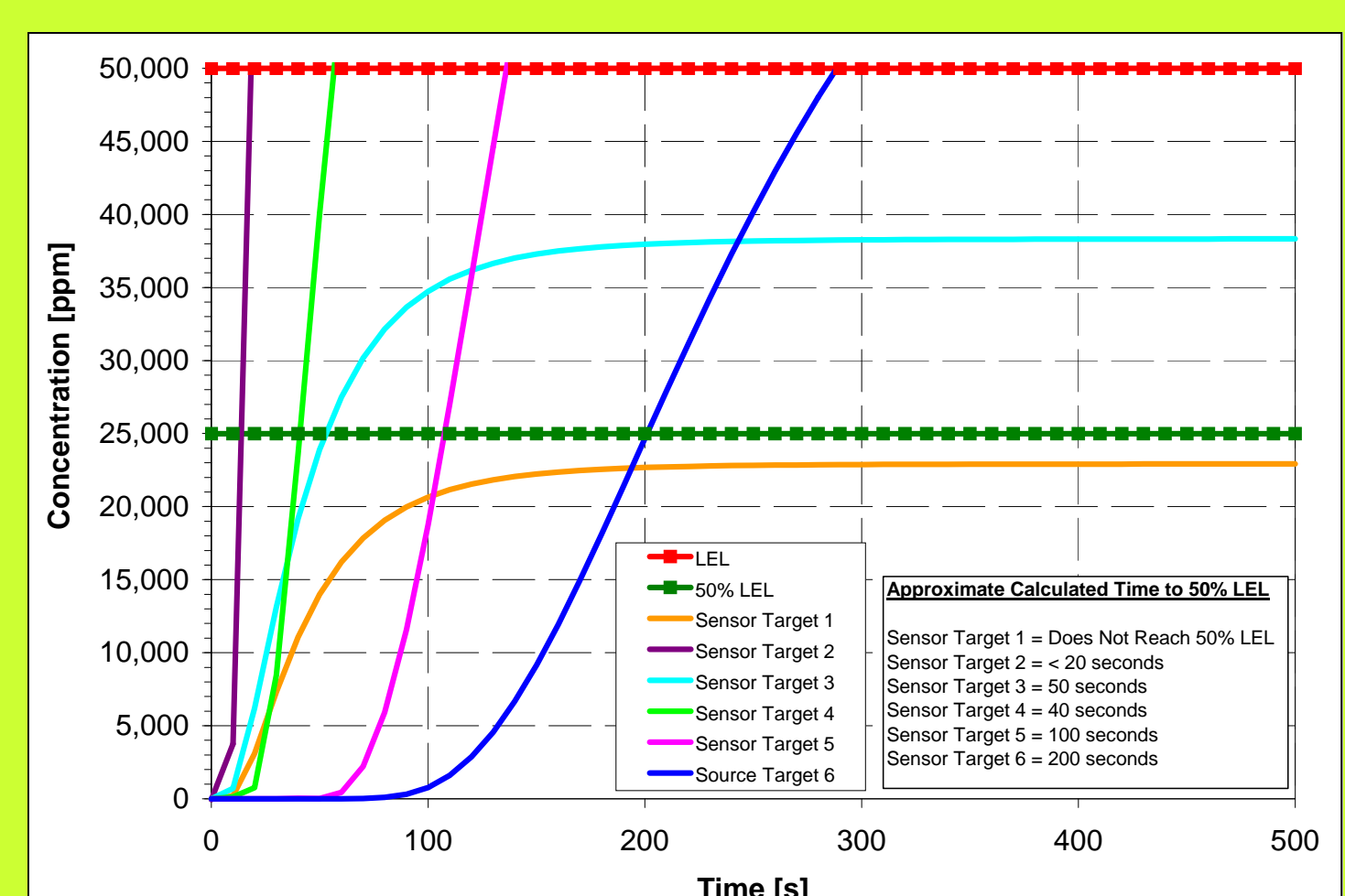


Figure 4. Predicted Methane Concentration Levels as a Function of Time for each of the Six Fixed Gas Detector Sensors.

## Case 3: Onshore CO Release

Using the same computational model, wind direction & wind profile as Case 2, HazRes has simulated a single release of Carbon Monoxide (CO) rich gas from the top of the same gas holder location.

HazRes used its CFD Gas Dispersion model to conduct a transient time-dependent analysis on the CO release relative to a target CO concentration which corresponds to significant Carboxyhemoglobin (COHb) level.

Some results of the transient CO gas discharge and dispersion analysis can be seen in **Figure 5** for 10 to 100 seconds from the start of release.

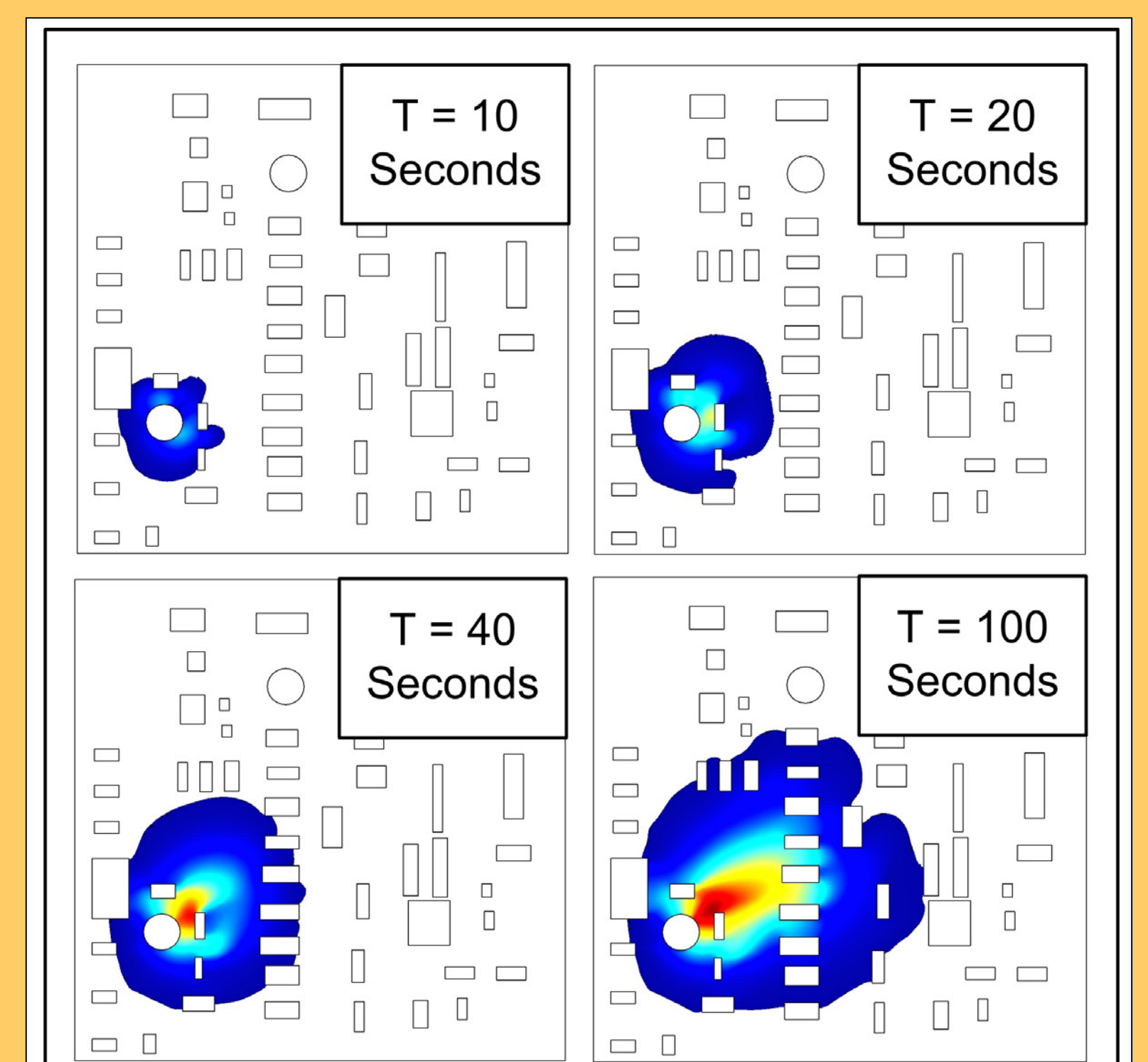


Figure 5: 2D Slice Plot at 3m Height Showing CO Dispersion as a Function of Time.