

# Predicting the Atmospheric Dispersion of Carbon Dioxide Releases from Pipelines for CCS Applications using CO2FOAM

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# Work Objectives

- Develop a predictive tool for the far field dispersion of released carbon dioxide (CO<sub>2</sub>) using computational fluid dynamics (CFD) techniques.
- Validate the predictions with full scale test data generated in the National Grid CO<sub>2</sub> PipeLine TRANSPORTation (COOLTRANS) research programme.
- Use the validated CFD tool to investigate the effects of topography/slopes and obstacles on the far-field dispersion of the released CO<sub>2</sub>.

# CO<sub>2</sub>FOAM

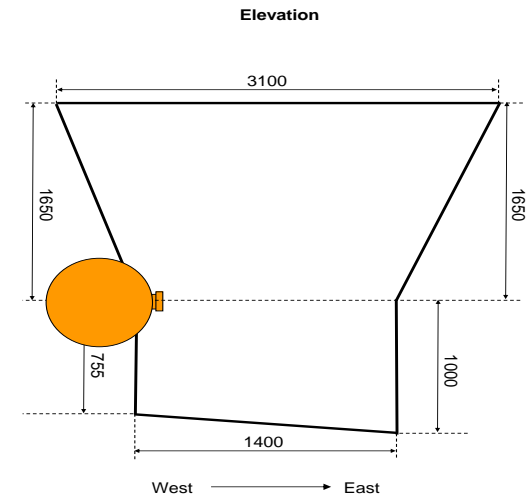
- **CO<sub>2</sub>FOAM** – a dedicated solver for CO<sub>2</sub> dispersion in the framework of the open source CFD code OpenFOAM®
- Two options for CO<sub>2</sub> dispersion:
  - The Homogeneous Equilibrium Model (HEM)  
*Jennifer Wen, Ali Heidari, Baopeng Xu and Hongen Jie, Dispersion of carbon dioxide from vertical vent and horizontal releases—A numerical study, Proc IMechE Part E: J Process Mechanical Engineering 227(2), 125-139, May, 2013.*
  - **The Homogeneous Relaxation Model (HRM)**

# CO<sub>2</sub>FOAM with HRM

- Mixture equations accounting for all phases.
- A relaxation model is employed to handle the presence of solid CO<sub>2</sub> within the release and its continuing sublimation.
- Buoyancy effects are important and included.
- Unsteady Reynolds Averaged Navier Stokes (RANS) approach.
- k- $\omega$  SST turbulence model for Reynolds Stresses.

# Experiment for Model Validation - Dense Phase Puncture Experiment (Case Study 3) in COOLTRANS Research Programme

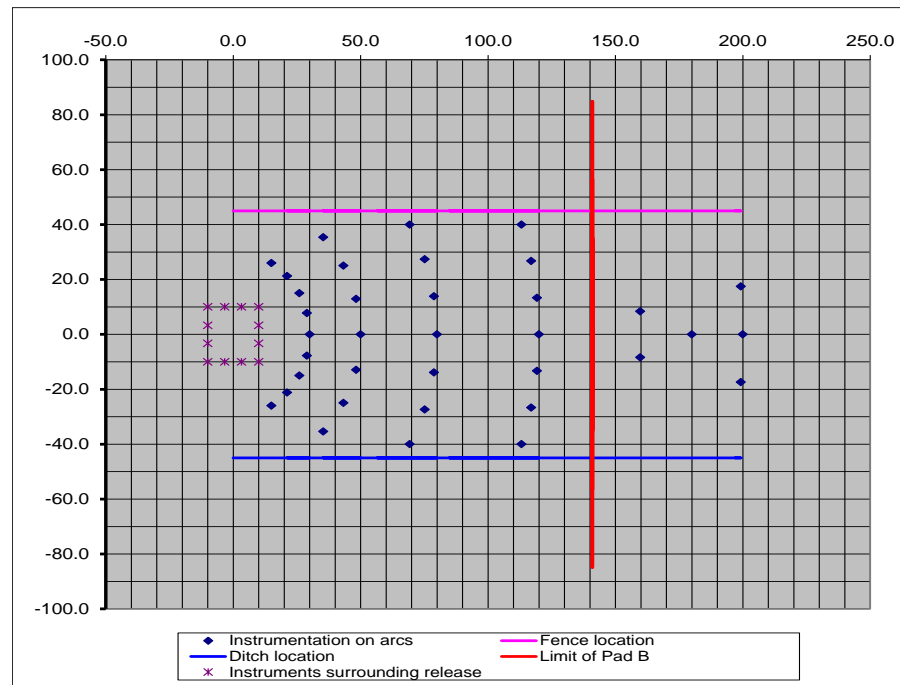
- A length of pressurised pipeline was used as the 'test section'.
- The CO<sub>2</sub> is released into the simulated crater.
- Liquid/gas CO<sub>2</sub> leaves the pipeline.
- Solid CO<sub>2</sub> formed within the crater due to Joule-Thomson effect.
- ~30kg/s of CO<sub>2</sub> leaves the crater, max. velocity ~23m/s.



NG PUNCTURES TEST08: Pre-formed Crater Details

A cross-section of the pre-formed crater through the point of release constructed to surround the release location in Case Study 3 of the COOLTRANS research programme (reproduced from Allason et al. (2012)).

# Experiment for Model Validation - Dense Phase Puncture Experiment (Case Study 3) in COOLTRANS Research Programme (Continued)



Locations of external temperature and concentration measurements in Case Study 3 (reproduced from GL (2011)).

# Computational Set Up

## Computational domain

Length	300 m
Width	200 m
Height	60 m
Total number of computational cells	2.8 M

## Boundary Conditions

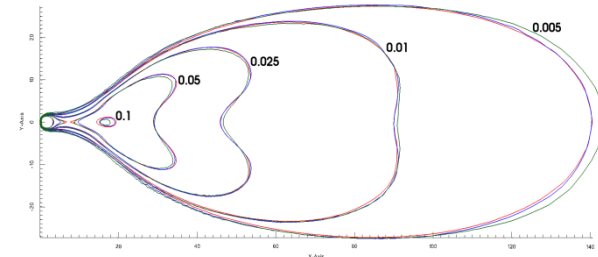
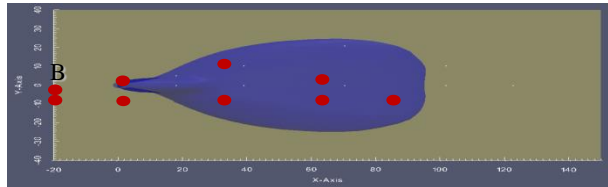
- Log profile at inlet.
- Constant shear stress at the top.
- Wall functions based on  $z_0$  for the ground.
- Zero gradient conditions on the sides.
- Values at crater exit plane taken from the near-field predictions of the University of Leeds calculations, both gas and solid CO<sub>2</sub> present.

# Mesh Sensitivity Study

## • Percentage Differences

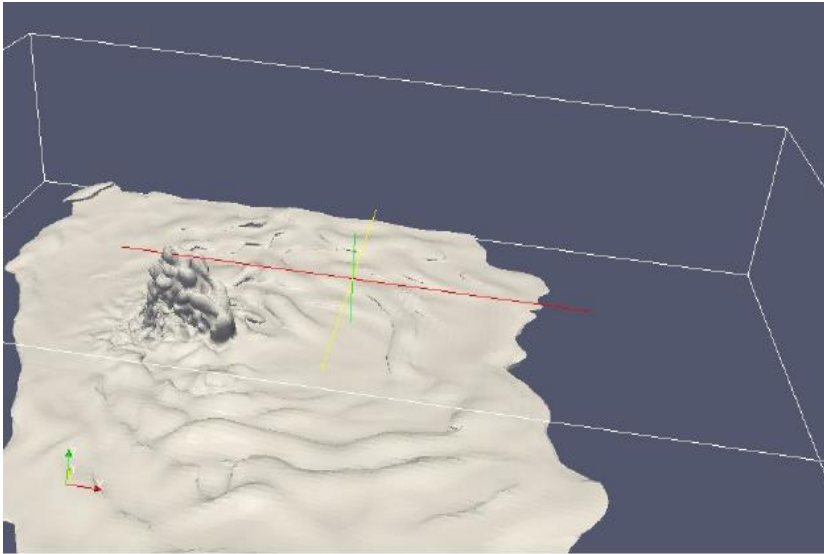
Points	$\beta$ at 3m height			$\frac{\beta_{coarse} - \beta_{middle}}{\beta_{middle}}$ %	$\frac{\beta_{fine} - \beta_{middle}}{\beta_{middle}}$ %
	coarse	middle	fine		
A	0.062	<b>0.063</b>	0.062	-0.92	-2.06
B	0.014	<b>0.013</b>	0.014	+6.92	+6.02
C	0.016	<b>0.016</b>	0.016	+2.24	+0.18
D	0.018	<b>0.019</b>	0.018	-3.45	-1.67
E	0.010	<b>0.010</b>	0.010	+1.60	+0.43
F	0.007	<b>0.007</b>	0.007	-2.14	-1.09
G	0.007	<b>0.007</b>	0.007	+1.00	+0.44
H	0.007	<b>0.007</b>	0.007	+0.63	-0.01
I	0.005	<b>0.005</b>	0.005	+0.47	+0.45

— coarse  
— medium  
— fine





# Overall Behaviour of the CO<sub>2</sub> Cloud



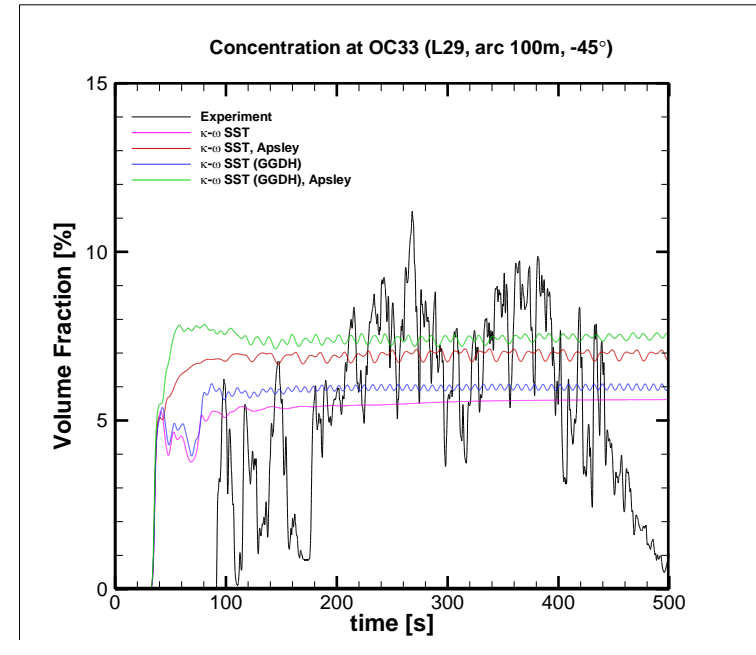
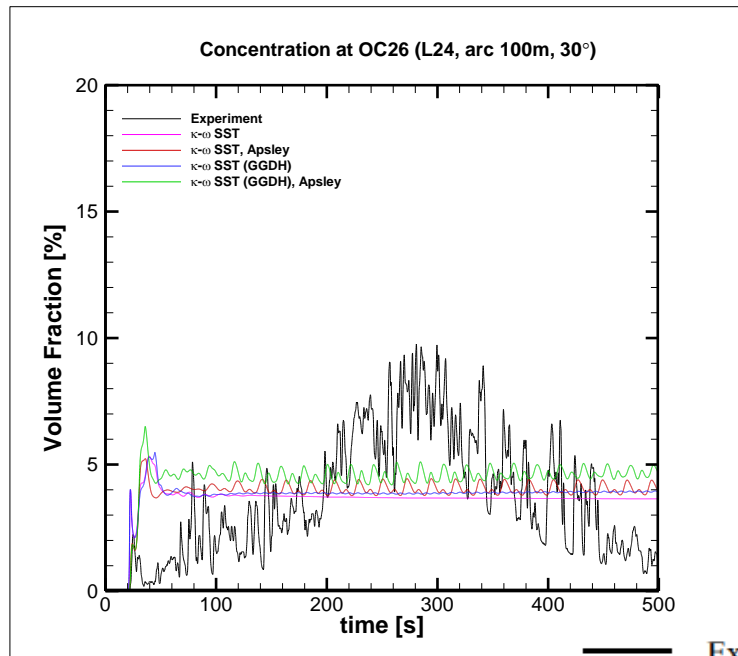
(a)



(b)

Overall view of mean concentration contours  $\beta = 1\%$  at different times (a) earlier and (b) later times.

# Comparison between the Measured and Predicted CO<sub>2</sub> Concentrations by Various $K-\omega$ SST Models



Experiment

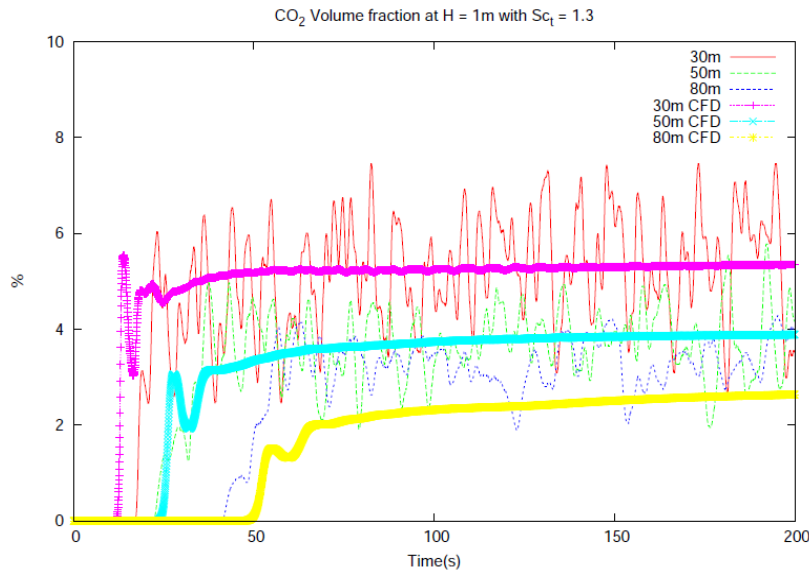
$k-\omega$  SST

$k-\omega$  SST, Apsley

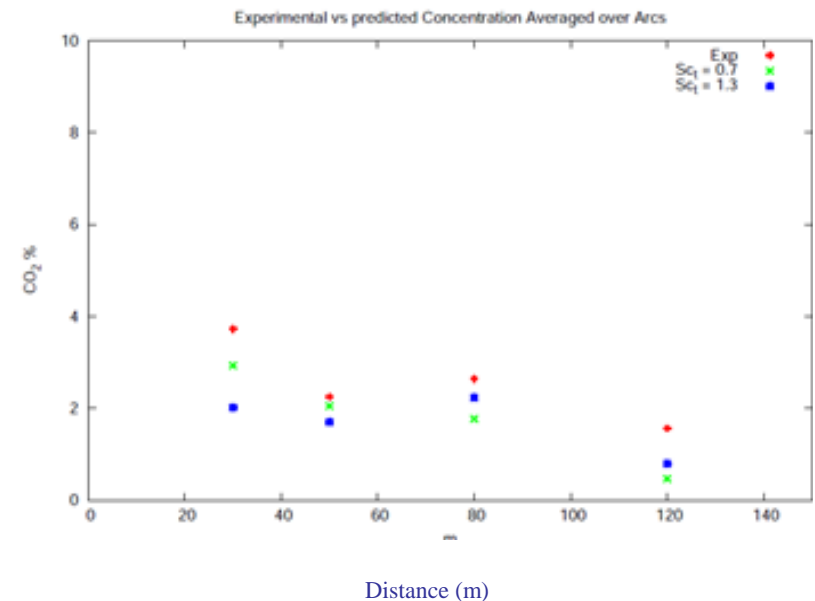
$k-\omega$  SST (GGDH)

$k-\omega$  SST (GGDH), Apsley

# Further Comparison between the Measured and Predicted CO<sub>2</sub> Concentrations



Comparison between the predicted and measured CO<sub>2</sub> volume fraction.



Comparison of the predicted and measured CO<sub>2</sub> concentrations averaged over the instrumentation arcs.

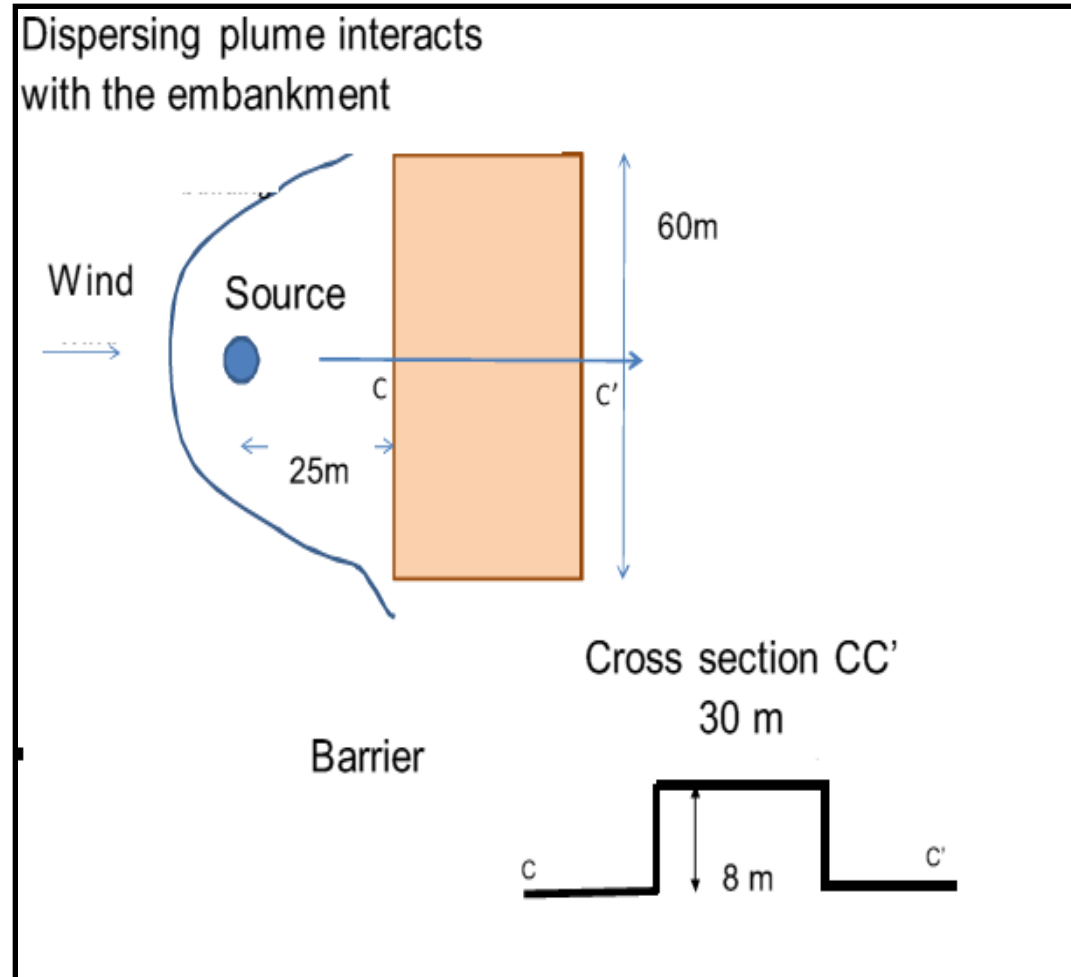
# Summary of CO<sub>2</sub>FOAM Validation

- The earlier slides show that the CO<sub>2</sub>FOAM can simulate a real event (e.g. a puncture) with reasonable accuracy.
- In the next few slides, a whole range of situations which were not covered in detail in the experiments are investigated with the 'validated' CFD model to see what is the predicted impact on the CO<sub>2</sub> behaviour.
- It should be noted that the examples do not necessarily reflect what would be allowed in practice, but were selected to examine the flow behaviour.

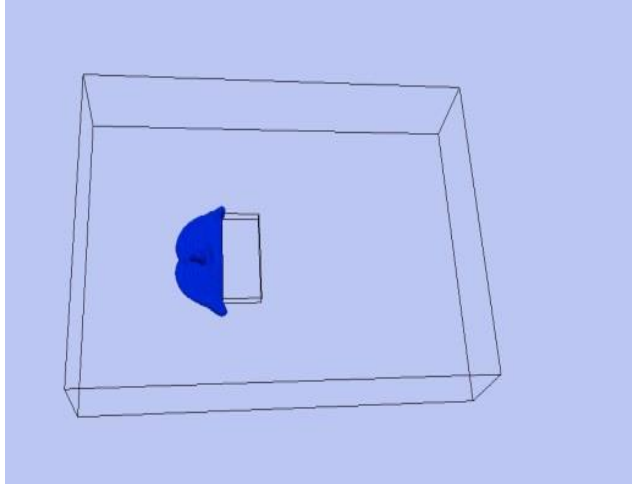
# The Effects of Obstacles

Four cases have been simulated in wind conditions of 1 m/s and 10 m/s:

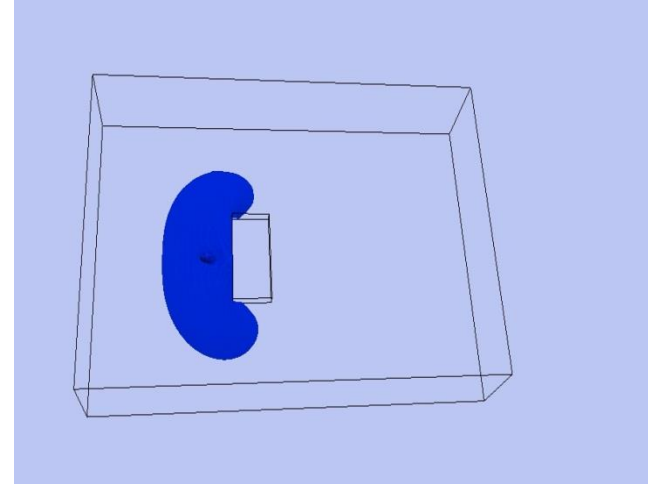
1. Flood defence.
2. Commercial building.
3. Domestic house.
4. Domestic house over a sloping terrain.



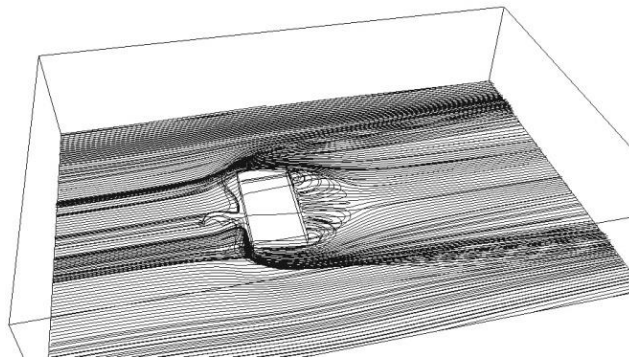
# The Effects of a Commercial Building



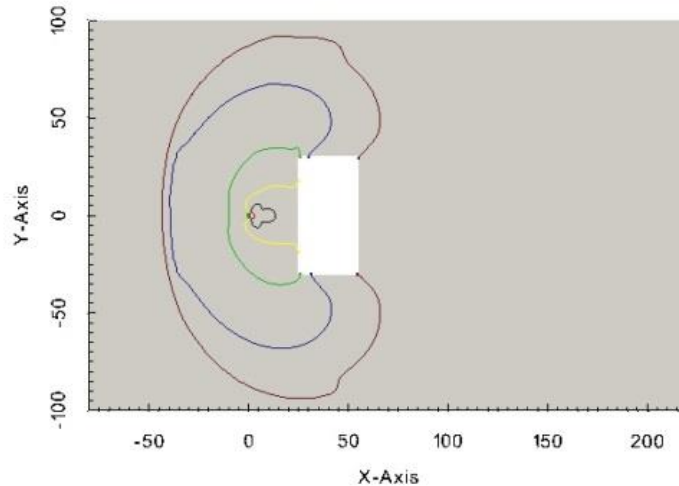
The predicted 2% CO<sub>2</sub> iso-contour  
at t = 30 s.



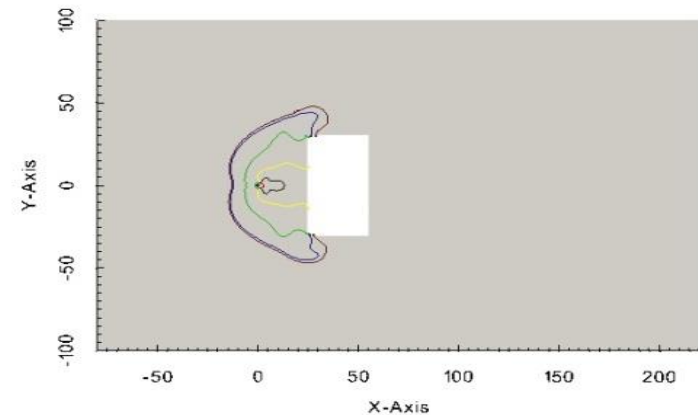
The predicted 2% CO<sub>2</sub> iso-contour  
at t = 300 s.



# The Effects of a Commercial Building (continued)



Horizontal CO<sub>2</sub> concentration profile at 1 m height and 30 s. Red: 20 %, black: 10 %, yellow: 7%, green: 4%, blue: 1.5% and brown: 0.5%.



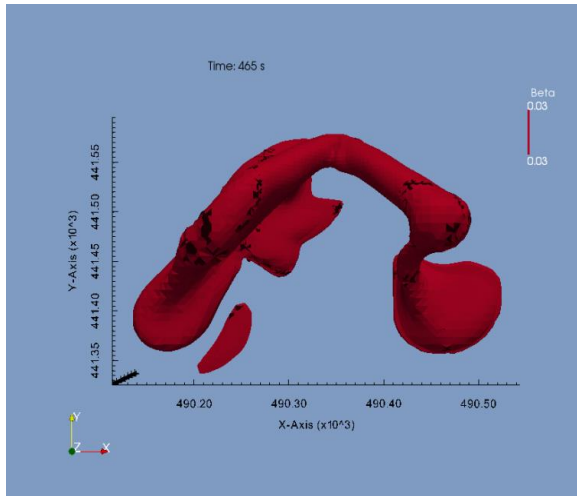
Horizontal CO<sub>2</sub> concentration profile at 1 m height and t = 300 s. Red: 20 %, black: 10 %, yellow: 7%, green: 4%, blue: 1.5% and brown: 0.5%.

# CO<sub>2</sub> Dispersion From Full Pipeline Rupture

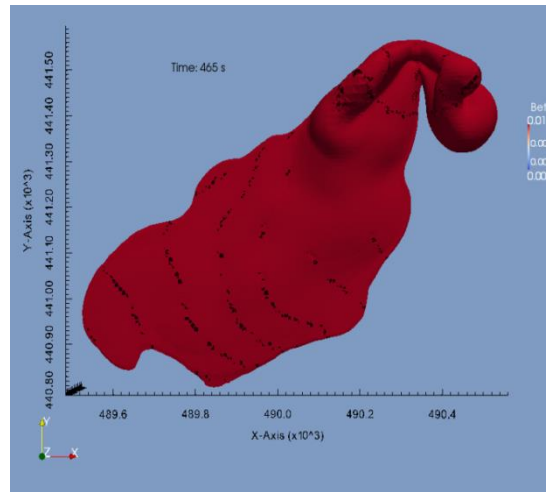
- The study used the release conditions of Case Study 5 in COOLTRANS. The near-field predictions from the University of Leeds are used as inlet conditions.
- The location of the rupture is assumed to be at the centre of the computational domain.
- Due to the high momentum of the release, the turbulence of the source dominates the atmospheric turbulence.
- Realistic terrain conditions are used as input to the geometry file.



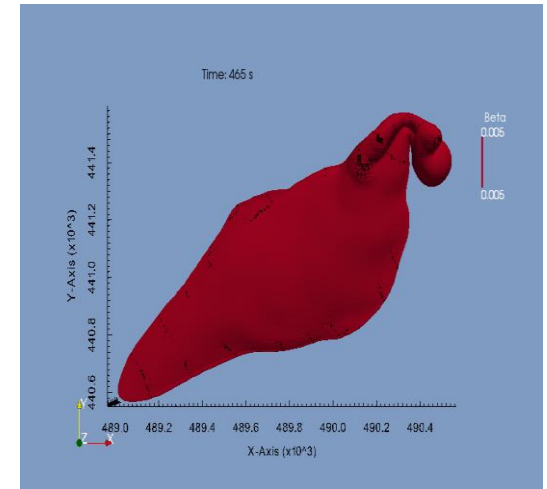
# Maximum Extent of Cloud after 465 s



(a)



(b)



(c)

CO<sub>2</sub> footprint: (a) 3% (b) 1% and (c) 0.5 % volume fraction iso-contours after 465 s.

# Concluding Remarks Concerning CO<sub>2</sub>FOAM

- CO<sub>2</sub>FOAM, a dedicated solver for CO<sub>2</sub> dispersion has been developed within the framework of OpenFOAM®
- Both the Homogeneous Equilibrium Model (HEM) and Homogeneous Relaxation Model (HRM) have been implemented to treat the multiphase flow conditions of CO<sub>2</sub>.
- Both Large Eddy Simulation (LES) and Reynolds Averaged Navier-Stokes (RANS) approaches are available.
- The predictions with the RANS approach with the *k- $\omega$  SST* turbulence model and ABL-specific wall-functions for a full scale puncture tests have achieved reasonably good agreement with the data in a blind validation.

# Concluding Remarks Concerning Obstacle and Terrain Effects

## Release 25 m in front of a commercial building:

- The building has both blocking and diluting effects to the CO<sub>2</sub> flow. The cloud can be trapped temporarily or diverted towards particular zones, potentially creating locally larger hazards in cases where there are open windows and doors. Higher concentrations (>4%) are constrained to upstream of the building.
- Locating a building 25 metres away from a release was a choice to investigate the effects of a building and was not used to see what is likely to happen in practice. The slide implies the extent of dilution that is predicted to happen in all cases. This was just an investigation of only one release and one building location and will not provide 'the answer' for all cases.

## Dispersion from full pipeline rupture in realistic terrain:

- The predictions show that the topography has considerable effects in the behavior of the released CO<sub>2</sub>. How these will affect the measures of harm will be further analyzed.