

# Experimental and Computational Evaluation of the Importance of Molecular Diffusion at Buncefield



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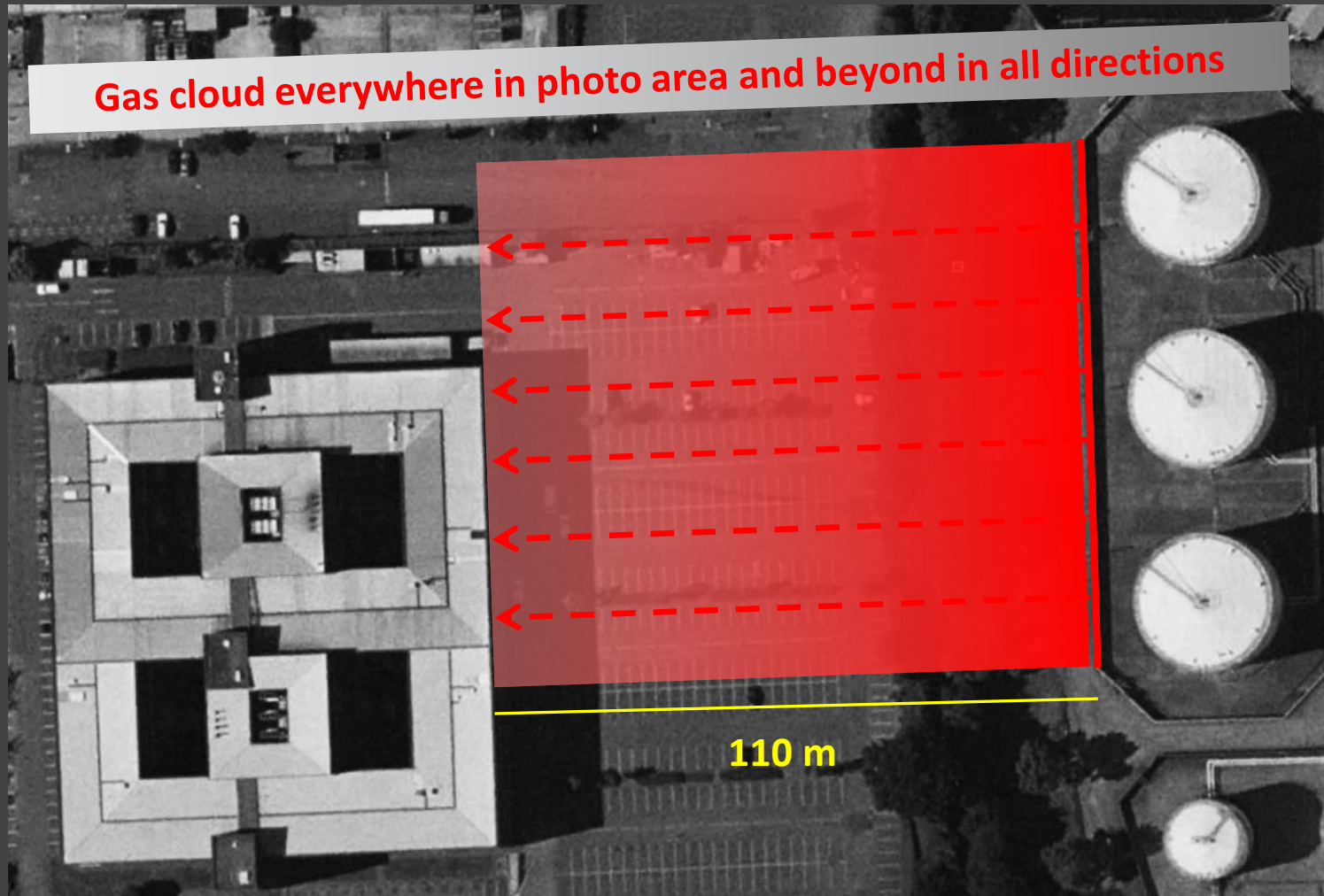
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**University of Arkansas**

**UKELG Workshop**

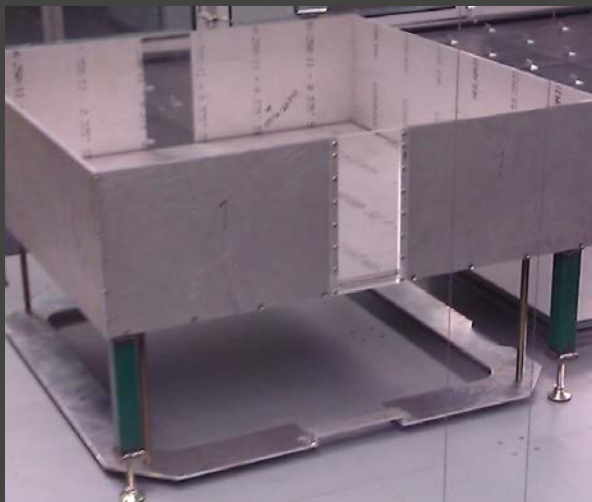
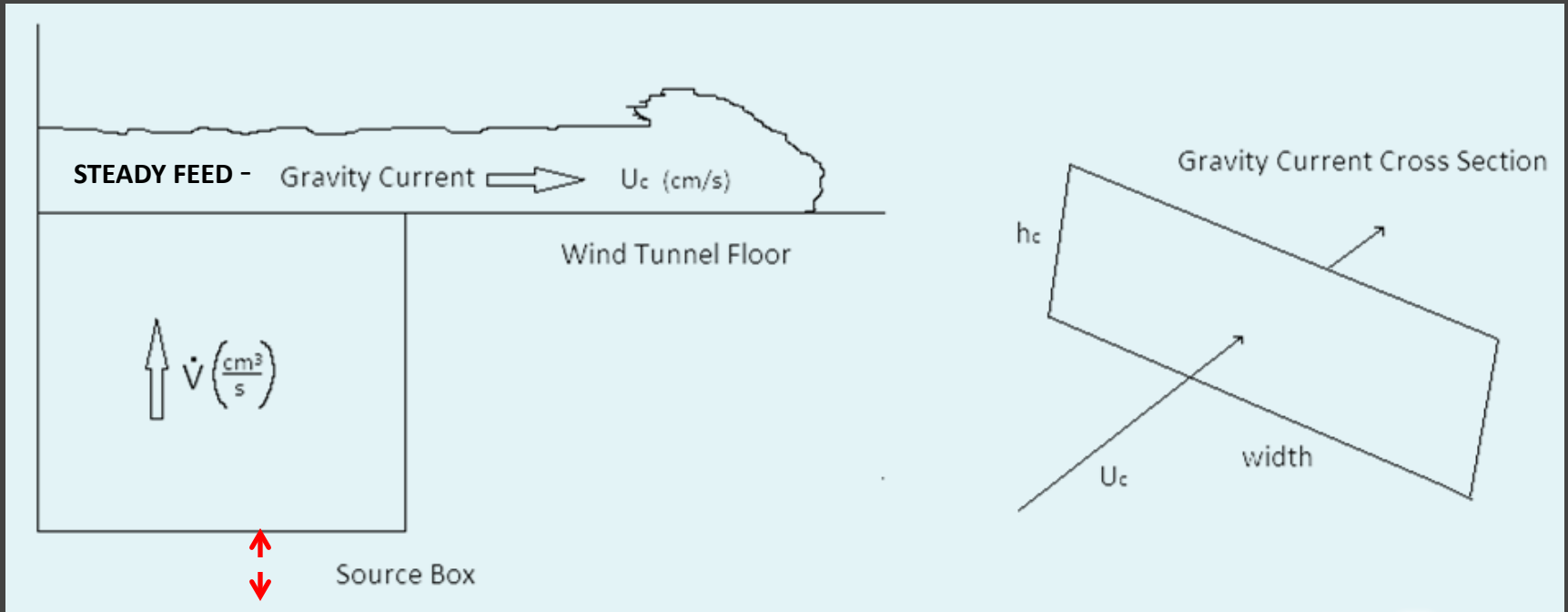
**Cardiff, Wales, July 2013**

# Assumed 2D Flow Area – Parking Lot Concentration Decreasing Right to Left



If we can understand and predict this approximately 2-D section's concentration dependence with time, can proceed numerically .....

# Experimental Design



- Reynolds Number

$$\frac{U_c h_c}{\nu}$$

- Froude Number

$$\frac{U_c^2}{g' h_c}$$

$\nu$  = kinematic viscosity,  $\text{m}^2/\text{s}$

$g' = g((\rho - \rho_{\text{air}})/\rho_{\text{air}})$ ,  $\text{m}/\text{s}^2$

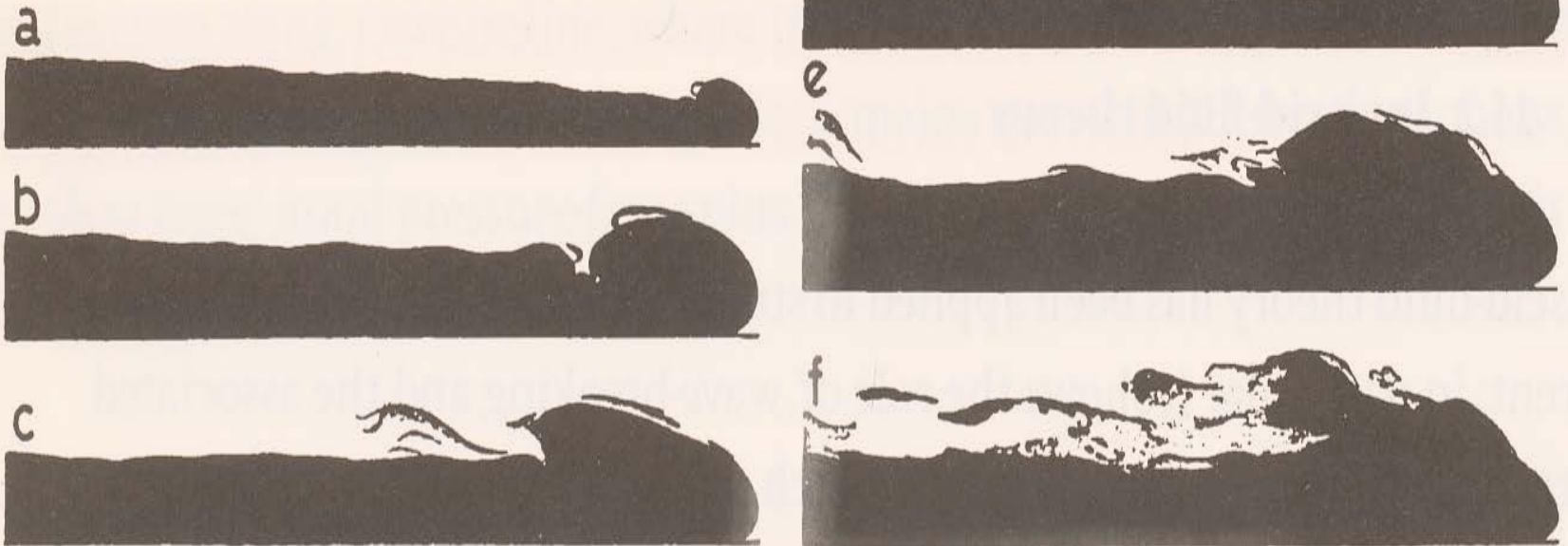
# Original Idea was to Investigate Reynolds Number Independence

- Model as steady-feed 2-D Gas Gravity Current (zero wind)
- Primary goal: measure gas concentration in the flow field
- Secondary goal: model a 2-D section of the Buncefield gas flow

## Liquid Gravity Currents

### Reynolds Number

increasing  $a(<10)$  –  $f(>1000)$



**Schmidt (1911) - Indicating “ $N_{re}$  Independence”**

# Original Idea

- Determine the Reynolds number required for  $N_{Re}$  independence and verify  $N_{Re}$  independence with concentration measurements.
- Measure the resulting non-dimensional concentration distribution in the “indicated” section of the Buncefield flow.

**BAD IDEA - ABANDONED**

# Path Forward

For the no-wind, density-stratified gas-gravity-currents under study, there appeared to be little, if any, meaning to the concept of Reynolds Number Independence except (possibly) as applying to the gravity current head. The gas gravity current behind the head appears to be essentially turbulence-free, in our experiments AS WELL AS IN THE BUNCEFIELD EVENT.

## Laminarization Criteria (from published literature)

Authors	Criterion
McQuaid (1976)	$U_m / (g \times g_o)^{1/3} < 3$
Stretch (1986)	$(g \times g') / U^3 > 0.005$
Britter (1989)	$(g' \times Q_o) / (U_*^3 \times W) > 0.1$
Hall & Waters (1989)	$(g' \times Q_o^{1/2}) / U^{2.5} > 1000$

where

$g$  = gravitational acceleration,  $m/s^2$

$g'$  = reduced gravitational acceleration,  $m/s^2$

$Q_o$  = volumetric flow rate,  $m^3/s$

$U$  = fluid velocity,  $m/s$

$U_*$  = friction velocity,  $m/s$

$W$  = bund perimeter,  $m$

# Revised Plan

Lab Expt  
and  
Buncefield  
Laminarization  
Criteria values

<u>Authors</u>	<u>Criterion</u>	<u>Expt/Buncefield</u>
McQuaid (1976)	$U_m / (g \times g_o)^{1/3} < 3$	0.79/0.73
Stretch (1986)	$(g \times g') / U^3 > 0.005$	2.0/2.5
Britter (1989)	$(g' \times Q_o) / (U^3 \times W) > 0.1$	2.0/2.3
Hall & Waters (1989)	$(g' \times Q_o^{1/2}) / U^{2.5} > 1000$	16329/87885

Design laboratory experiment for air mixing into the moving cloud by molecular diffusion only (minimize entraining head formation).

Develop and verify a model of the concentration field in the laboratory experiment

Predict concentration in the Buncefield flow (2D section of parking lot) assuming air mixing into the cloud limited to molecular diffusion



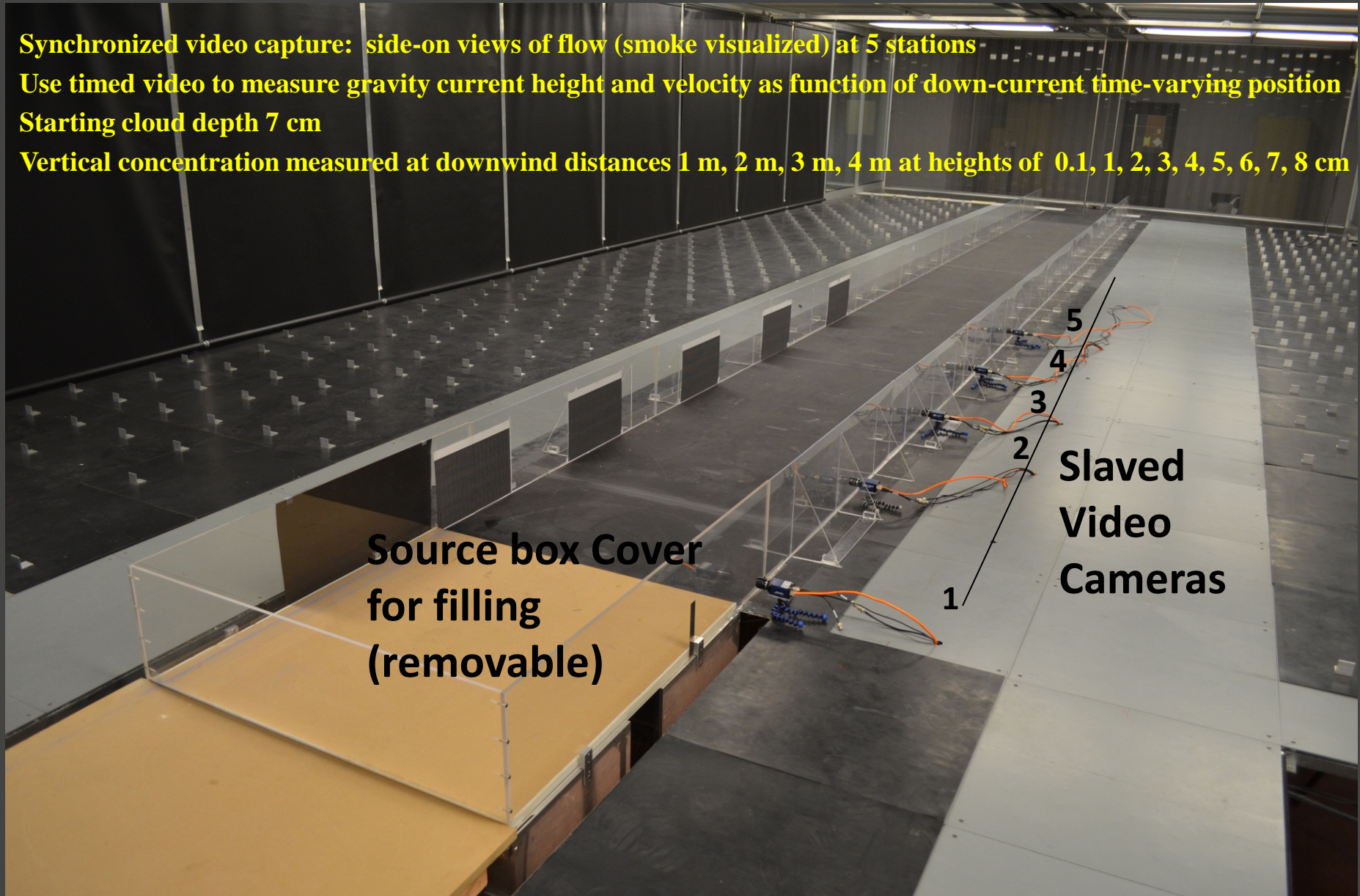
# Experiment Design

**Synchronized video capture: side-on views of flow (smoke visualized) at 5 stations**

**Use timed video to measure gravity current height and velocity as function of down-current time-varying position**

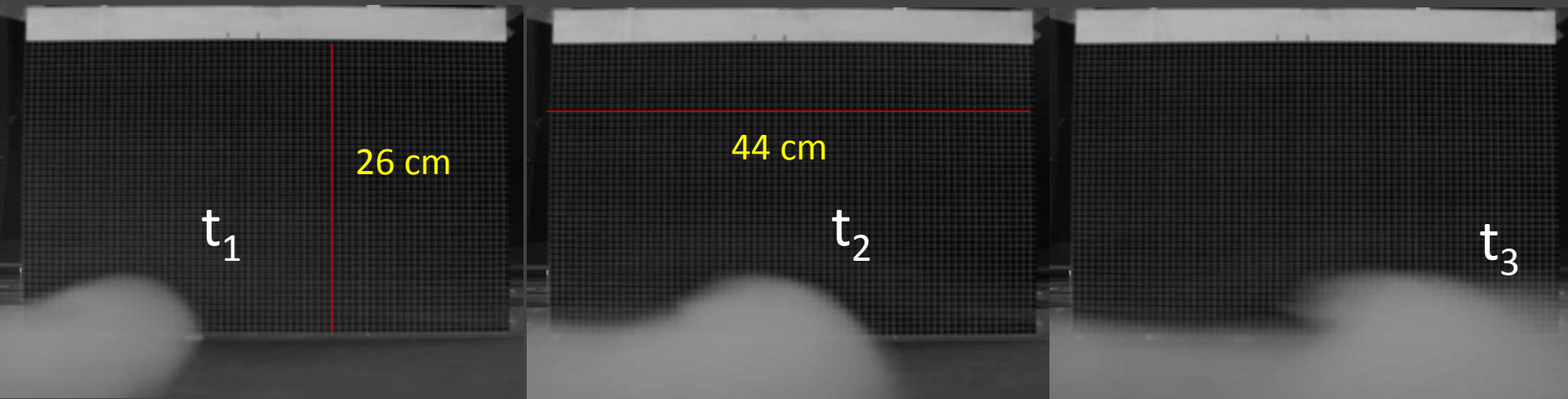
**Starting cloud depth 7 cm**

**Vertical concentration measured at downwind distances 1 m, 2 m, 3 m, 4 m at heights of 0.1, 1, 2, 3, 4, 5, 6, 7, 8 cm**





# Typical Timing Camera Frames Indicating Head Development



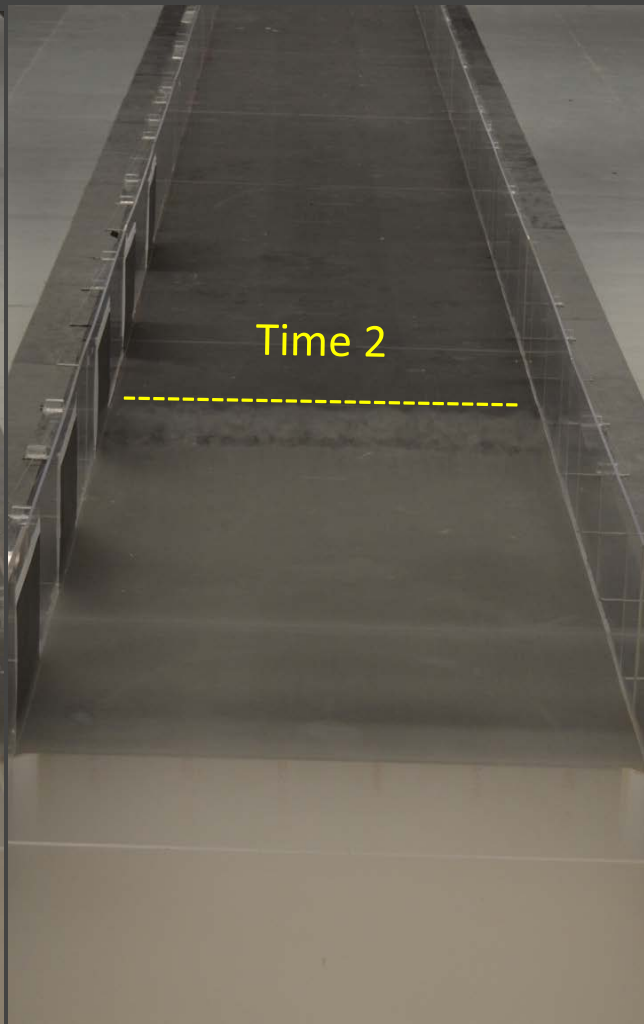
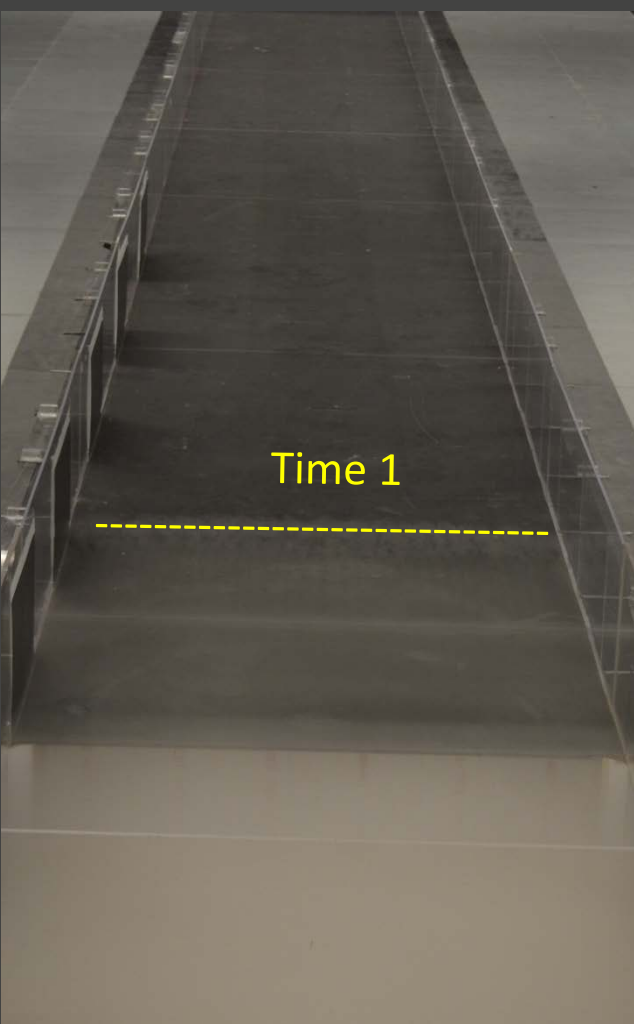
# Buncefild Density

Gas Density =  $1.35 \text{ kg/m}^3$

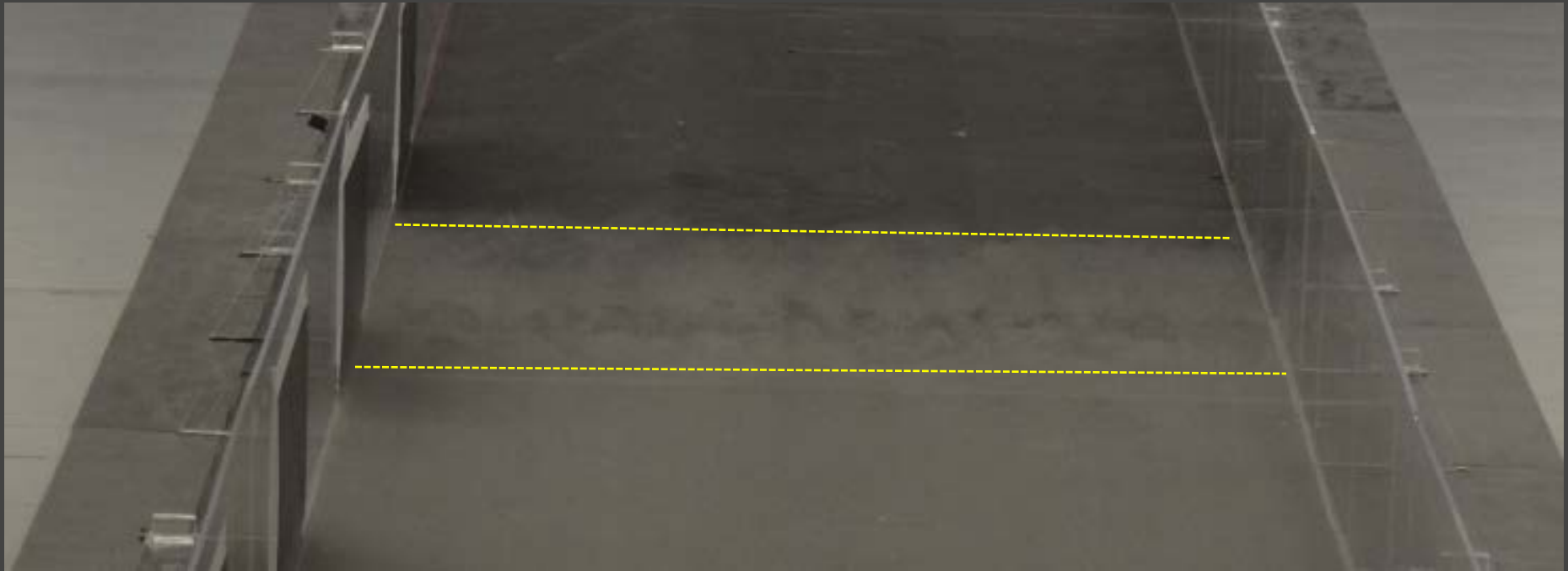
Height of Gas Layer Moving from Box = 8.4 cm

Height of 8.4 cm indicates  
Velocity of Current =  $15.3 \text{ cm/s}$

Box Edge



# Front Structure



# Lab Experiment Design

Density 1 =  $1.77 \text{ kg/m}^3$  “CO<sub>2</sub>” ( $g' = 4.87 \text{ m/s}^2$ )

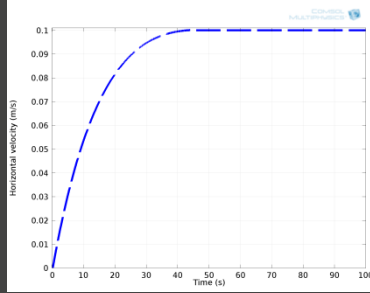
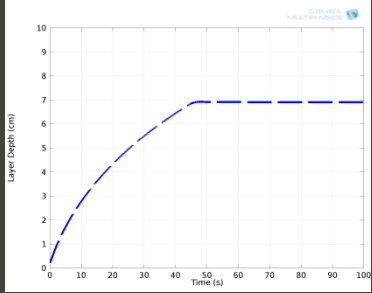
- For illustration, checks for consistency

Density 2 =  $1.35 \text{ kg/m}^3$  “Buncefield” ( $g' = 1.40 \text{ m/s}^2$ )

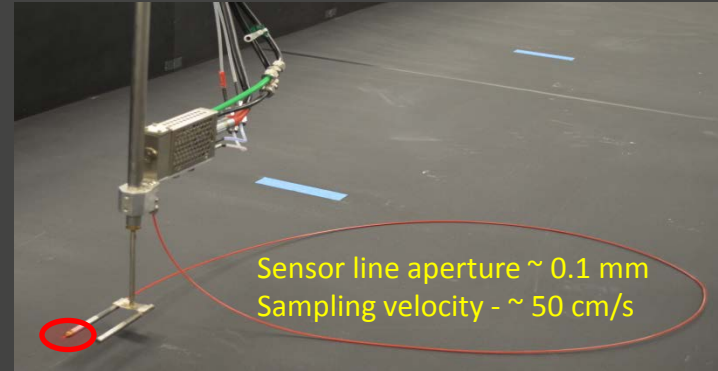
- Video records to measure timing
- Concentration measurements to define time-varying cloud concentrations - Measure gas concentrations with FID at specific heights and down-channel locations



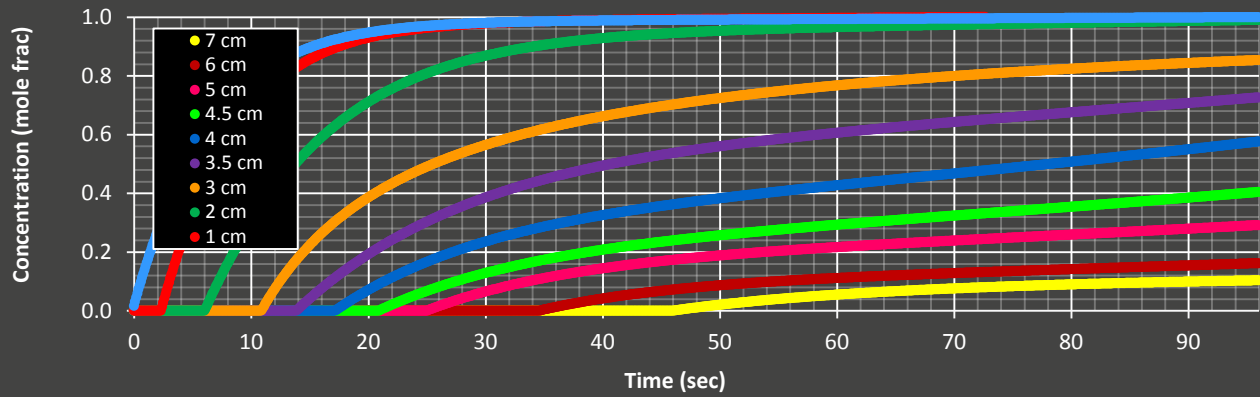
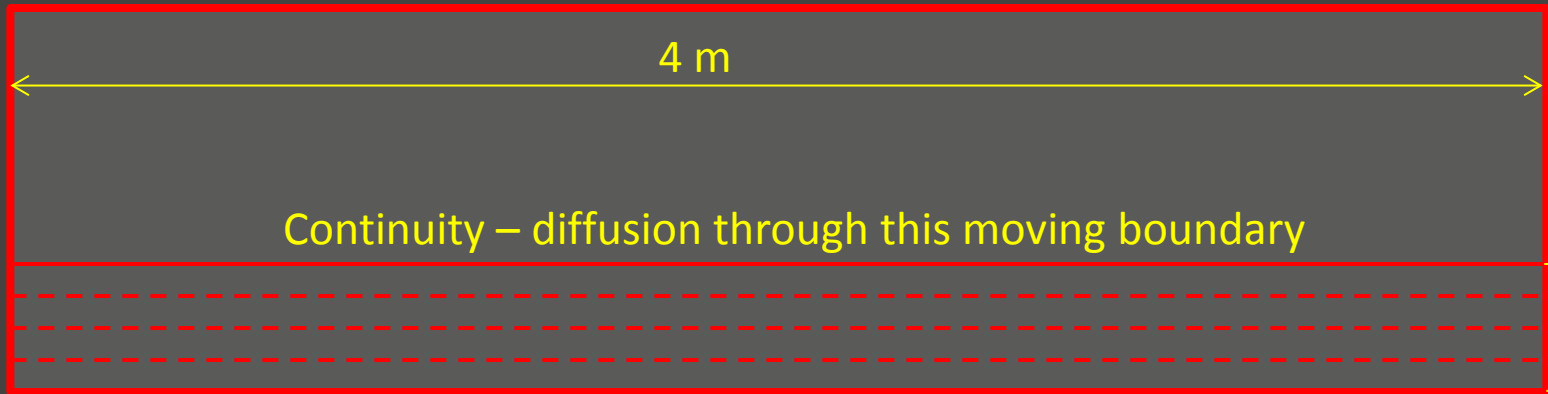
# Lab Experiment - Computational domain and boundary conditions



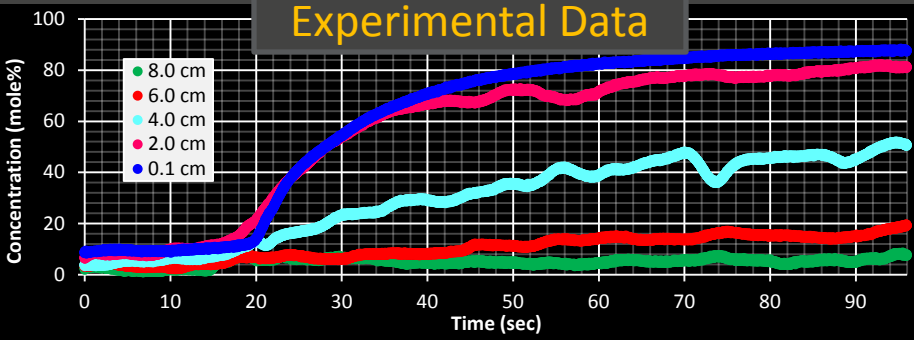
$C = 0$



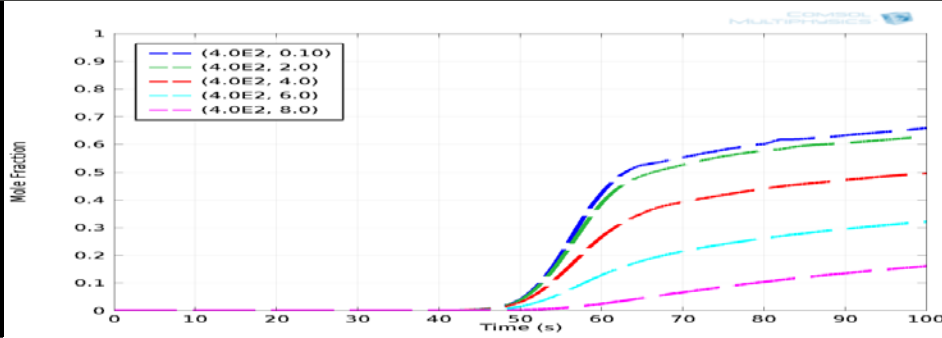
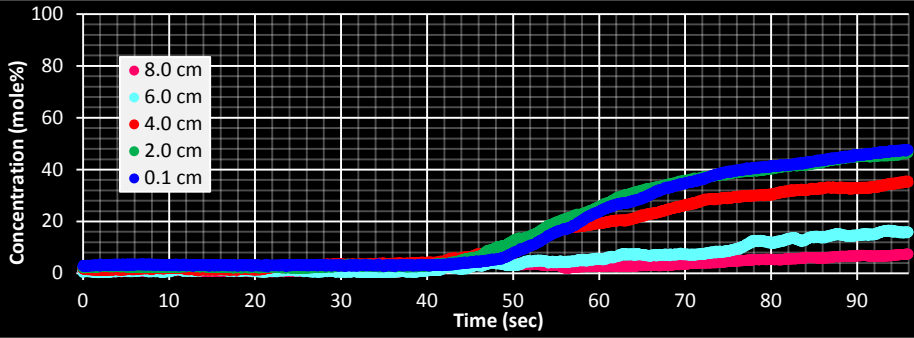
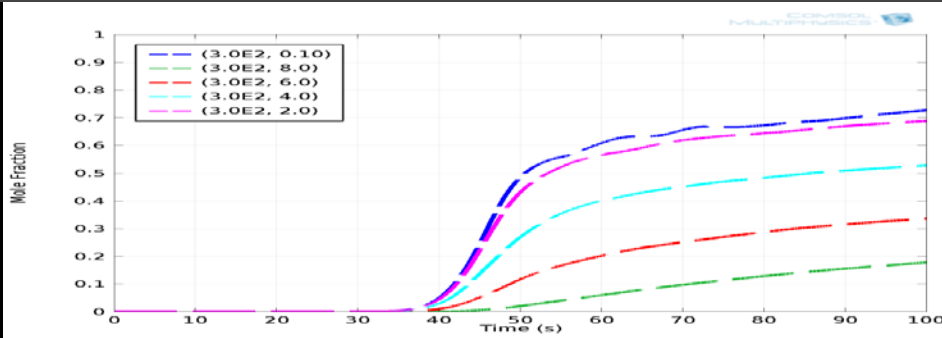
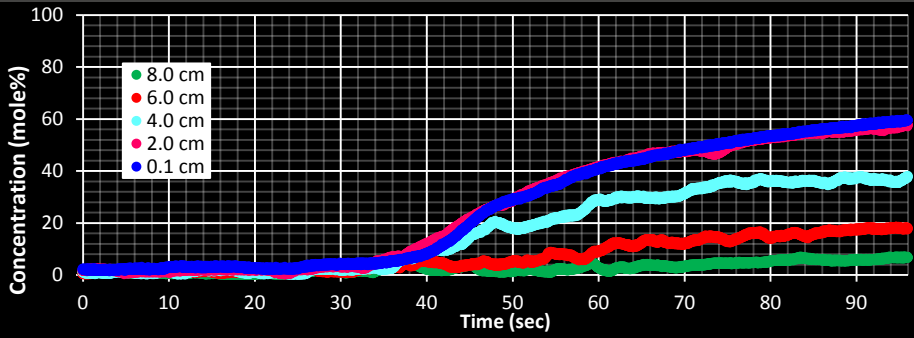
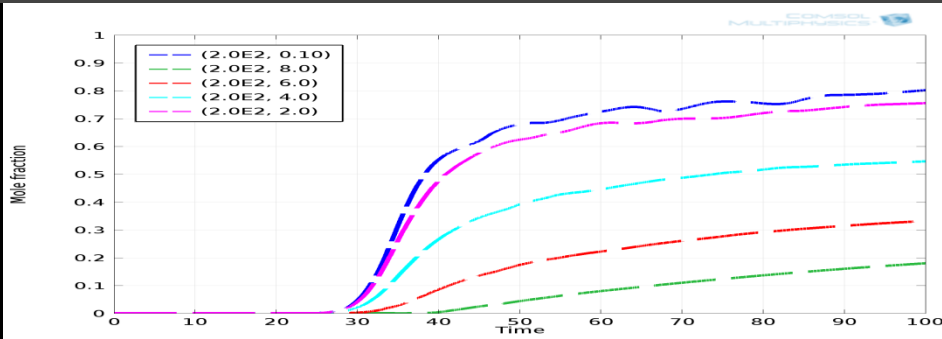
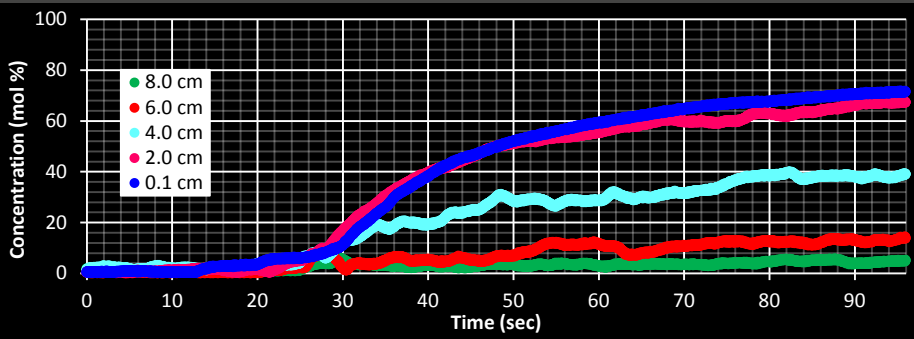
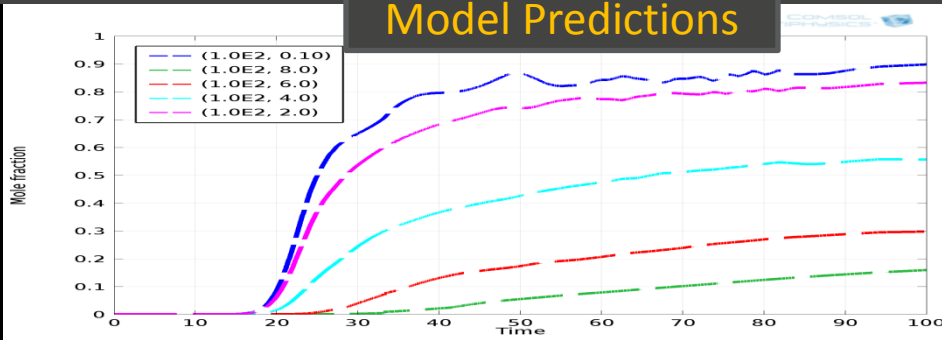
Inlet concentration and velocities



# Experimental Data



# Model Predictions

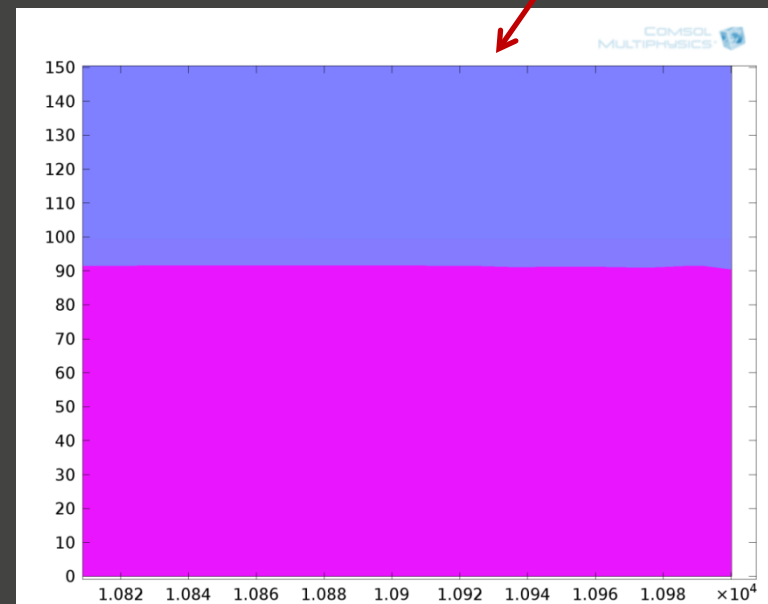
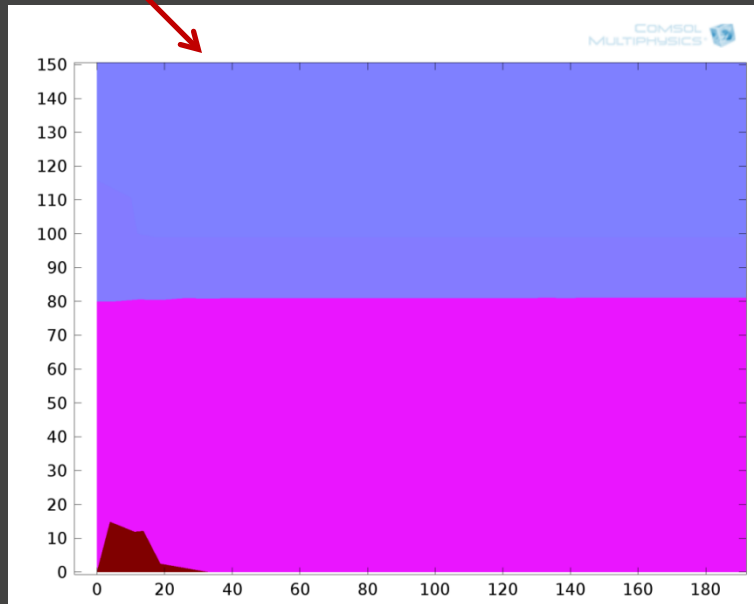


# Implications for Buncefield

Diffusion can act to increase the explosive volume!

110 m (300 s)

5 m



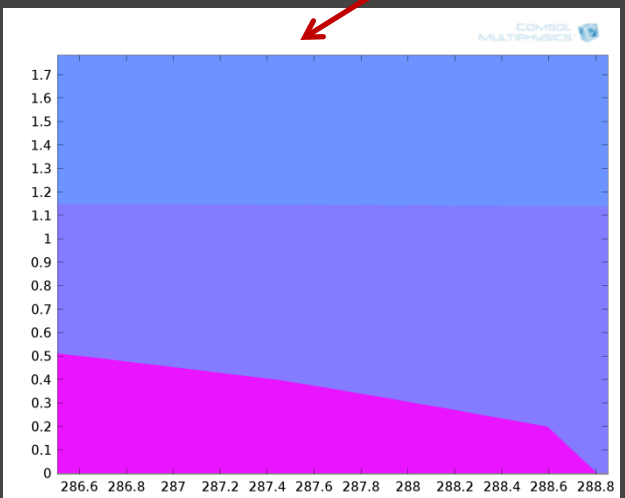
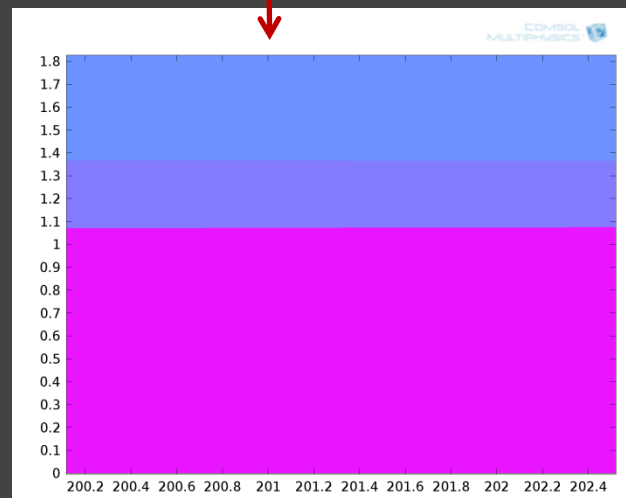
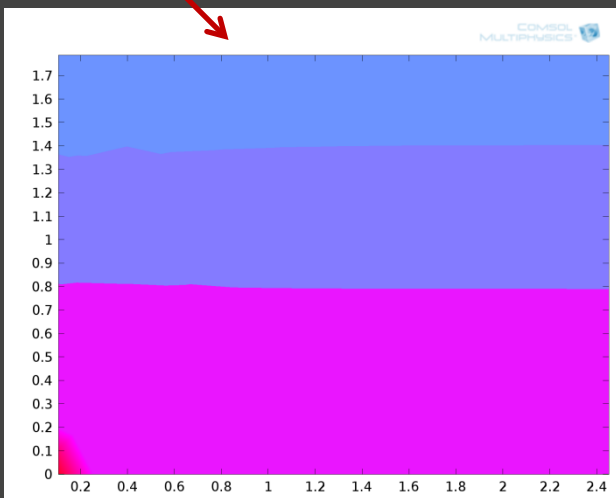
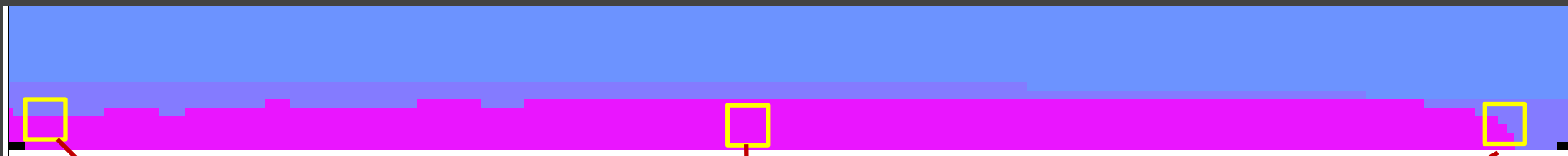
# Implications for Regulatory Modeling

HSE Considering model for determining range to which a circular cloud could be ignited.

$$R_{\text{ignition}} = [1/\rho V_{\text{cloud}} T]^{1/2}$$

For the example problem offered by HSE, we have calculated the effect of diffusion that would occur at the top of the cloud; the HSE model, which assumes no dilution, is conservative, but not overly so. However the explosive volume is indicated to increase.

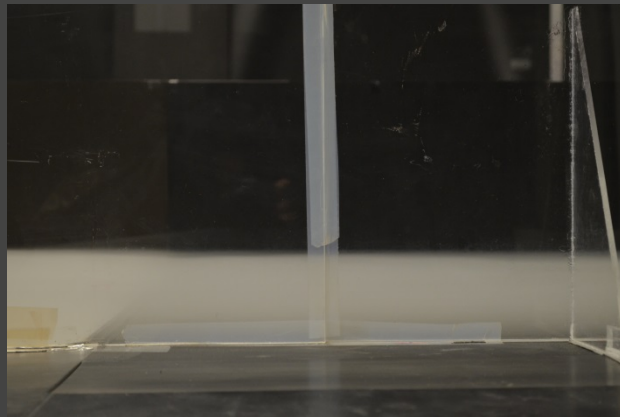
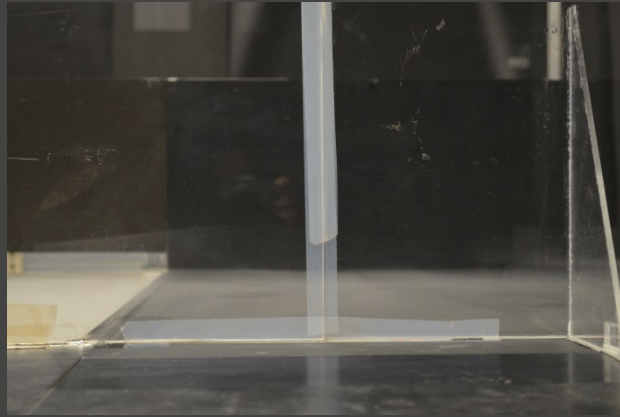
300 m (1400 s)



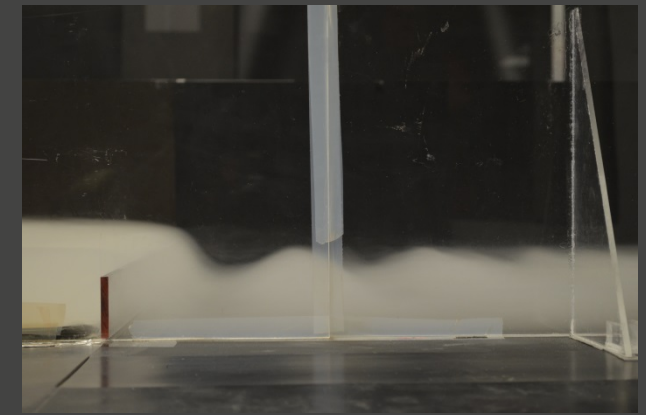
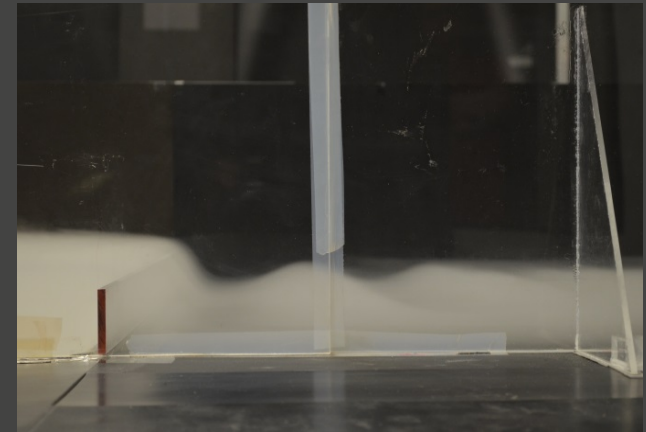
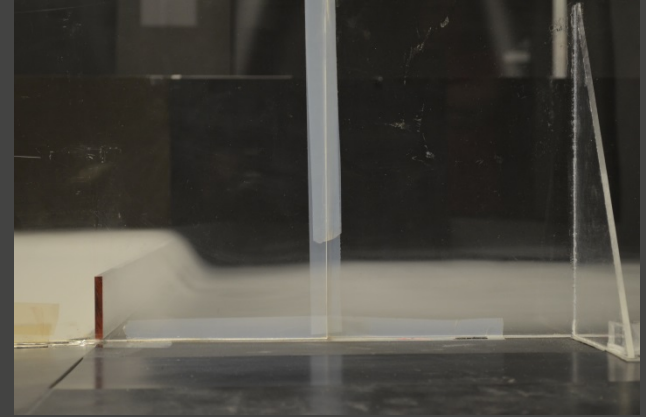
# Speculations Regarding Effect of Dikes

- Layer thickness develops faster without dike
- Thinner, but faster, layer resulting from overflow of dike, results in greater diffusion
- Complex wave effects probably not important

No Fence



Fence





# Conclusions

1. No-wind, shallow cloud depths, and long time scales indicate potential for important molecular diffusion effects.
2. Transient development of cloud thickness, starting concentration, and spreading velocity should be considered.
3. There is potential for diffusion effects to make concentrations more uniform and possibly increase potential for explosion.
4. Control measures for avoidance of such potential increases in hazard appear practical and worthy of consideration.