# Simulation of Hydrogen Dispersion under Cryogenic Release Conditions

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# OUTLINE

- Objectives
- Physics of LH2 dispersion
- Description of experiments
- Modeling Strategy
- Results
- Conclusions
- Future work

# OBJECTIVES

- Define safety zones in case of an accidental release of liquefied hydrogen (LH2) using CFD tools
  1. Understand physics of LH2 dispersion
  2. Develop the CFD code
  3. Validate the code
  4. Use CFD code for prediction in similar cases

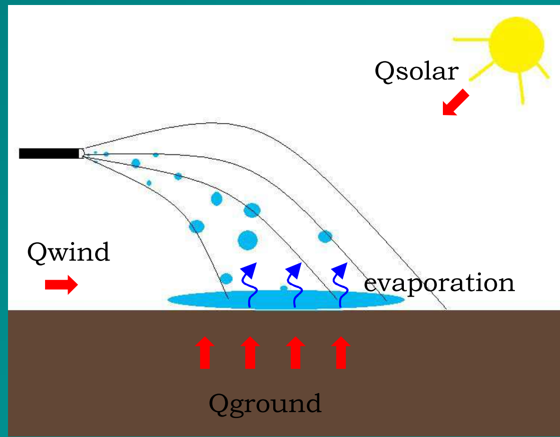
Validation of the ADREA-HF CFD code for cryogenic releases using the HSL experiments.

# Physics of LH2 dispersion

Two phase release → Two phase flow (vapor and droplets) + cryogenic pool is formed

During LH2 release:

- Cold cloud – Negative buoyancy
- Heat absorbing by the surrounding – Positive buoyancy




Factors that influence H2 dispersion:

- Release conditions
- Terrain features
- Atmospheric conditions
- Weather **conditions** (ambient temperature, ambient **humidity** wind velocity, **direction** etc.)
- Heat transfer from the ground

# Physics of LH2 dispersion

Presence of Humidity

Condensation\Solidification

Heat liberation Droplet and Ice crystals

- Air
- Vapor $H_2$
- Vapor $H_2O$
- Liquid $H_2$
- Liquid $H_2O$
- Solid $H_2O$

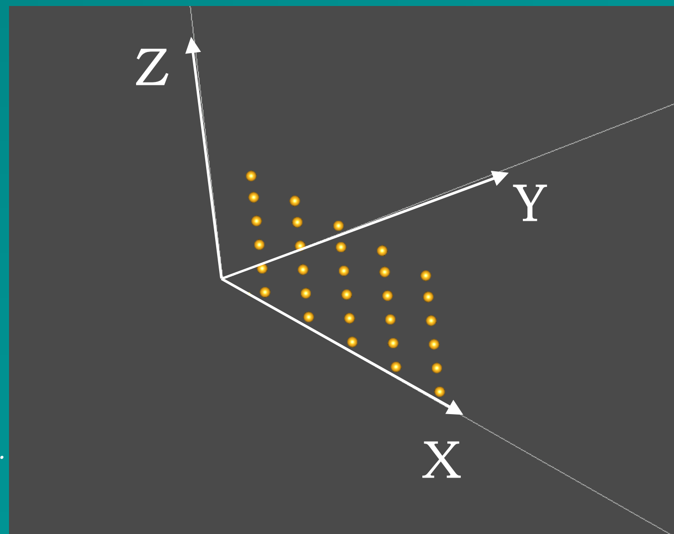
$\left.\begin{array}{l}\text{Liquid } H_2\\ \text{Liquid } H_2O\\ \text{Solid } H_2O\end{array}\right\}$ Non vapor phase

# Description of Experiments

Release and Weather Conditions for the simulating tests [1]

| Data / No test | 5 | 6 | 7 |
|---|---|---|---|
| spill rate (kg/sec) | 0.07 | 0.07 | 0.07 |
| spill diameter (mm) | 26.6 | 26.6 | 26.6 |
| source height (mm) | on ground (3.36) | 100 | 860 |
| source direction | Horizontal (x-direction) | Vertical (z-direction) | Horizontal (x-direction) |
| release duration (sec) | 248 | 556 | 305 |
| average wind speed (@2.5m) (standard deviation) | 2.675 *0.09* | 3.36 *0.95* | 3.07 *0.82* |
| average wind direction (@2.5m) (standard deviation) | 291 *15.5* | 295 *13.4* | 294.5 *14* |
| average ambient temperature (@2.5m) | 283 | 283 | 283 |
| ambient relative humidity (%) | 68 | 68 | 64 |

Experimental site (above) and sensors (below)




[1] *Hooker, P., Willoughby, D.B. and Royle, M., Example, Experimental Releases of Liquid Hydrogen, 4th International Conference on Hydrogen Safety, San Francisco, Paper 160, 2011.*

# MODELING STRATEGY

- Conservation equations: Non Equilibrium model / Hydrodynamic Equilibrium Model (slip terms)

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left((\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) + \rho g_i - \delta_{3i}\frac{\partial}{\partial z}\left(\rho q_{nv} w_s (1 - q_{nv}) w_s\right)$$

$$\frac{\partial \rho q_k}{\partial t} + \frac{\partial \rho u_j q_k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{Sc_t}\frac{\partial q_k}{\partial x_j}\right) - \frac{\partial \rho q_{nv} w_s (1 - q_k)}{\partial z}$$

$$\frac{\partial \rho H}{\partial t} + \frac{\partial \rho u_j H}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{Pr_t}\frac{\partial H}{\partial x_j}\right) + \frac{Dp}{Dt} + \frac{\partial}{\partial z}\left[\rho q_{nv} w_s (H - H_{nv})\right] - q_{nv} w_s \left(1 - \frac{\rho}{\rho_{nv}}\right)\frac{\partial P}{\partial z}$$

- Slip model[2]: $w_s = -31.21\left(\frac{\rho q_{nv}}{\rho_{H_2O}}\right)^{0.125}$
- Phase distribution: Non vapor phase of component-I appears when the mixture temperature falls below the mixture dew temperature, which is calculated using the Raoult's law for ideal gases. The solid phase of component-I appears when the mixture temperature drops below the freezing point.
- Standard k-ε with buoyancy effect term.
- One dimensional, transient energy (temperature) equation inside the ground. The ground consists of two layers (an upper concrete layer and a sand layer on the bottom).

[2] *Ogura Y. and Takahashi T., Numerical Simulation of the Life Cycle of a Thunderstorm Cell, Monthly Weather Review Journal, 99, 1971, pp. 895-911*

# MODELING STRATEGY

Simulation process:

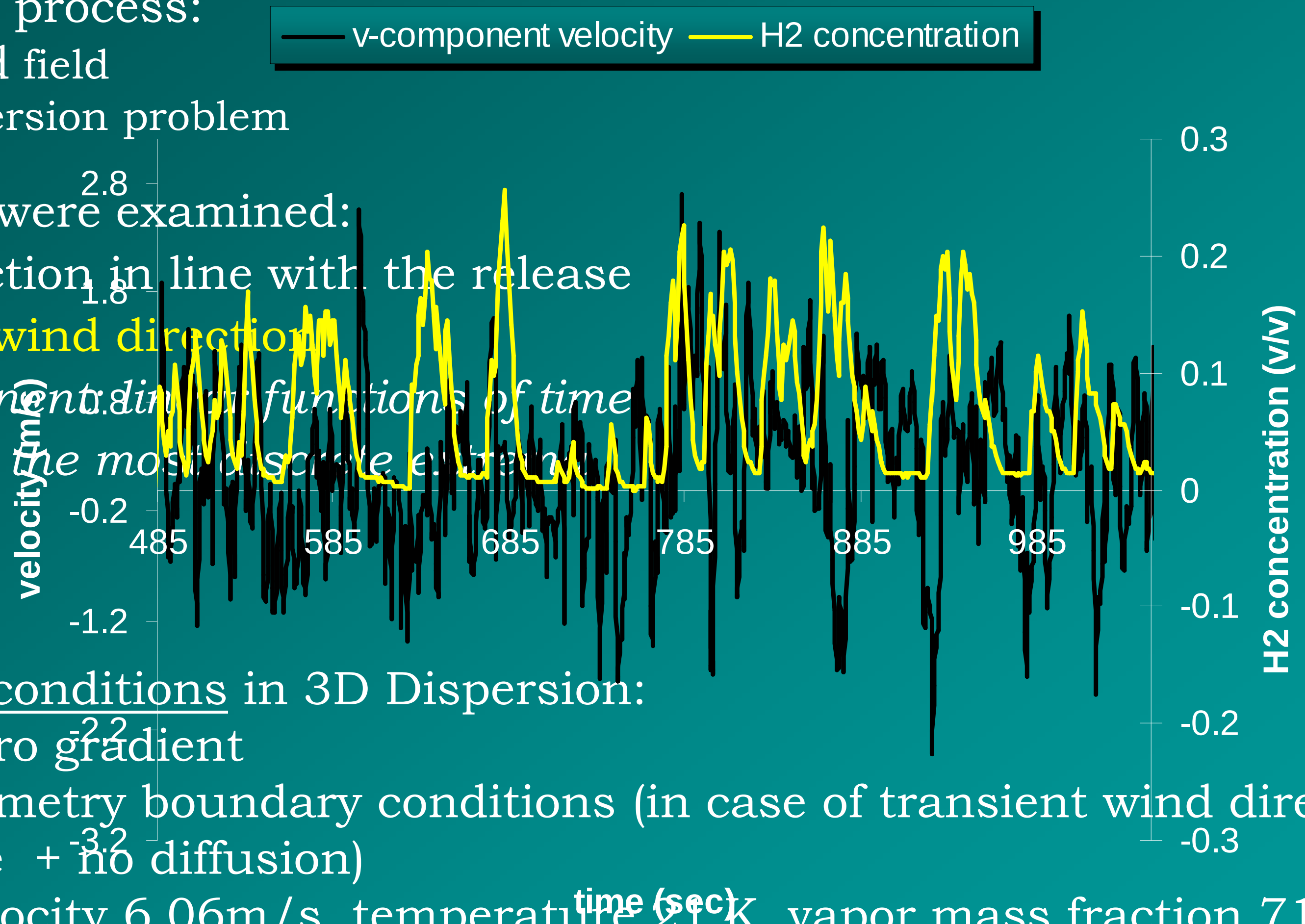
1. 1D wind field
2. 3D Dispersion problem

Two cases were examined:

-wind direction in line with the release

-transient wind direction

*v-component: linear functions of time between the most discrete extrema*




Boundary conditions in 3D Dispersion:

Outlet – zero gradient

Side – symmetry boundary conditions (in case of transient wind direction given value + no diffusion)

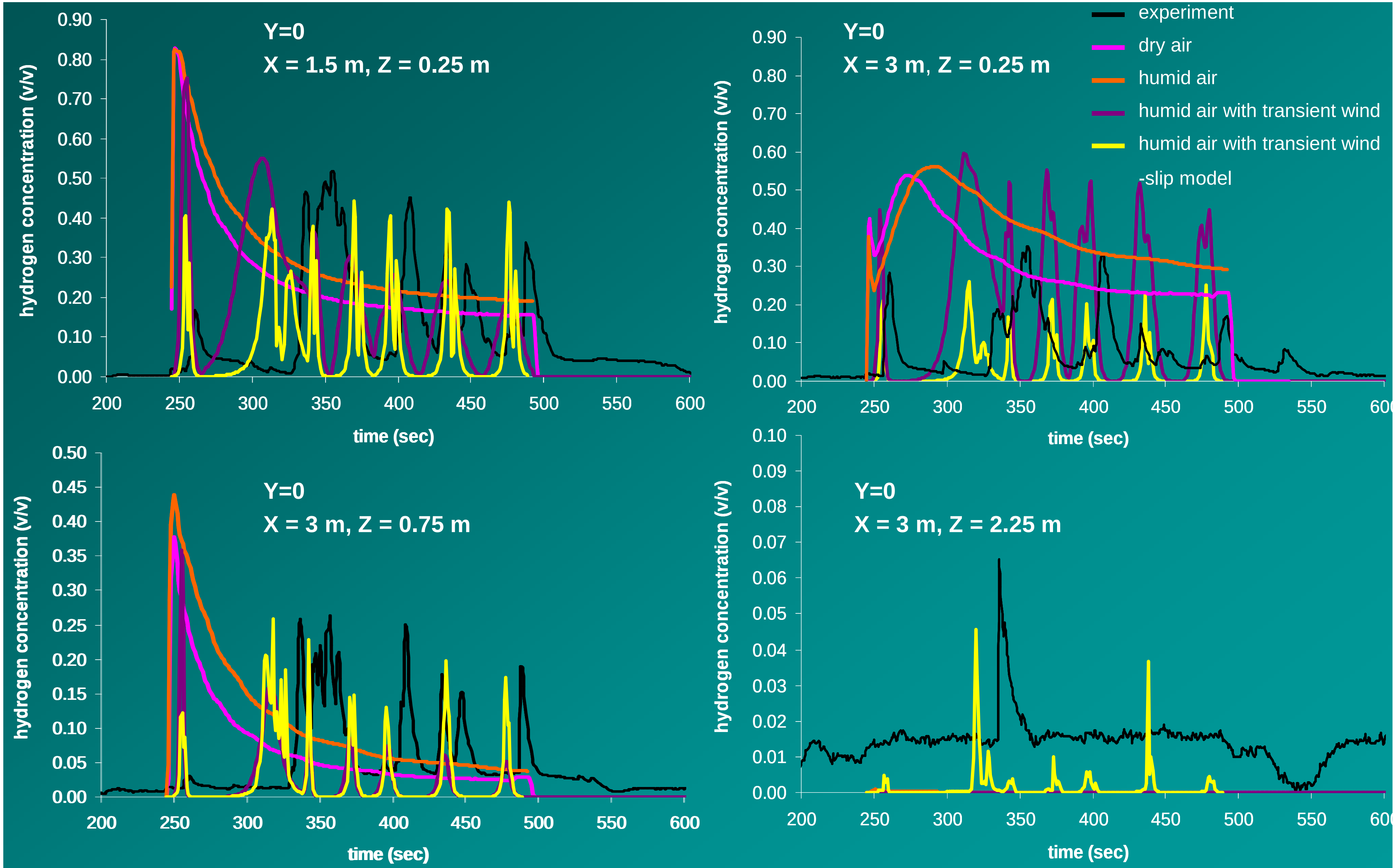
Source: velocity 6.06m/s, temperature 21 K, vapor mass fraction 71.34%

Test 6 - vertical release

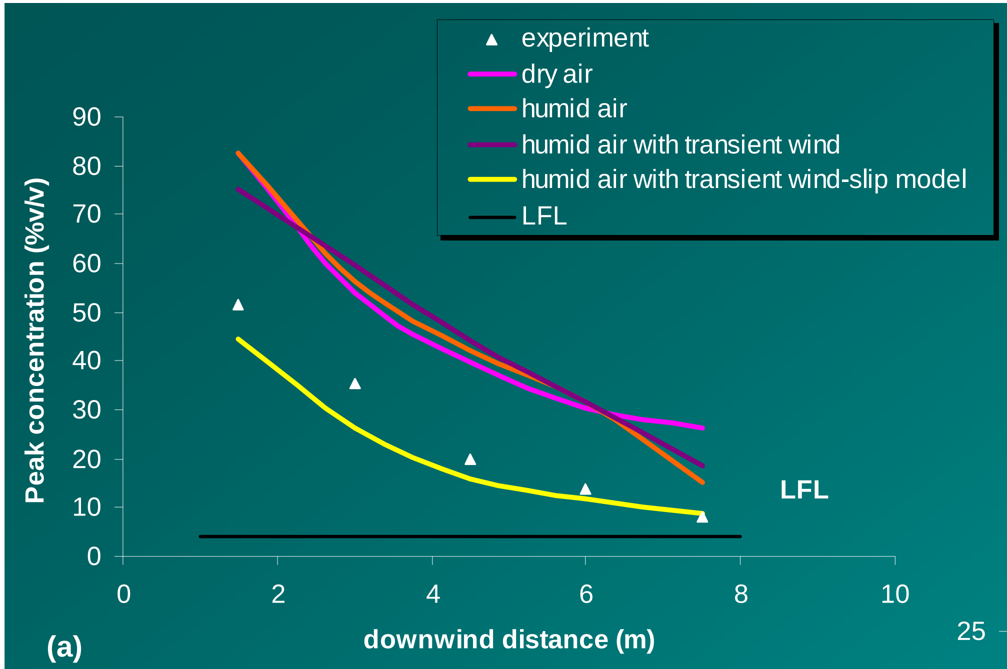
# MODELING STRATEGY

| | Computational domain (m) (x, y, z) | Grid Characteristic (m) | | | | |
|---|---|---|---|---|---|---|
| | | grid dimension | total number of cells | dx min | dy min | dz min |
| **Test5** | (15, 20, 10) | 40 x 69 x 34 | 93 840 | 0.1 | 0.027 | 0.027 |
| **Test6** | (15, 20, 10) | 63 x 68 x 28 | 119 952 | 0.027 | 0.027 | 0.05 |
| **Test7** | (25, 20, 10) | 45 x 69 x 49 | 152 145 | 0.1 | 0.027 | 0.027 |

# RESULTS (TEST 5)

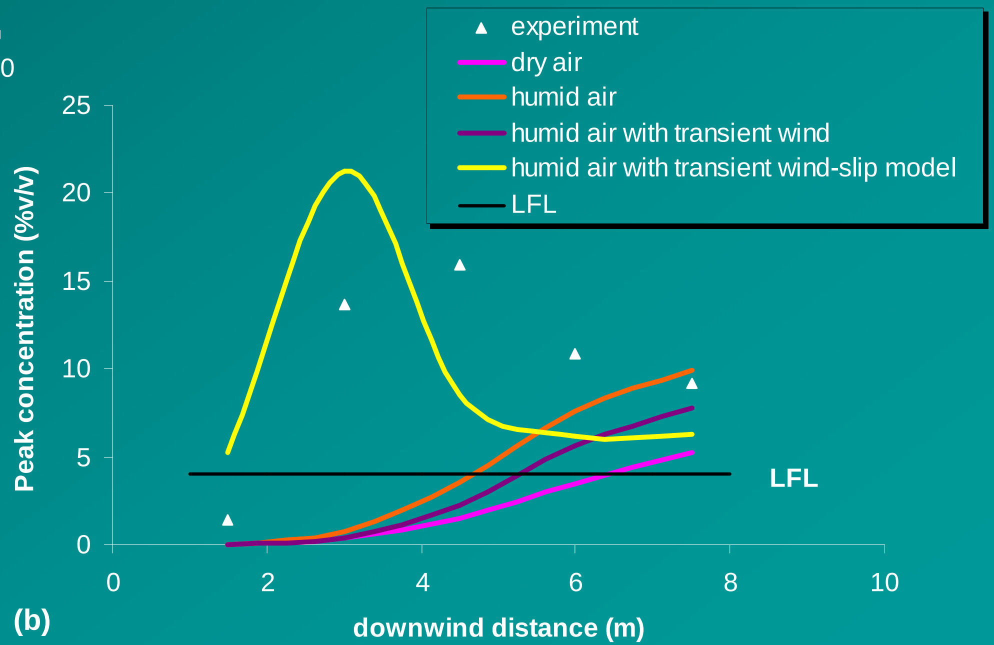


# RESULTS (TEST 5)

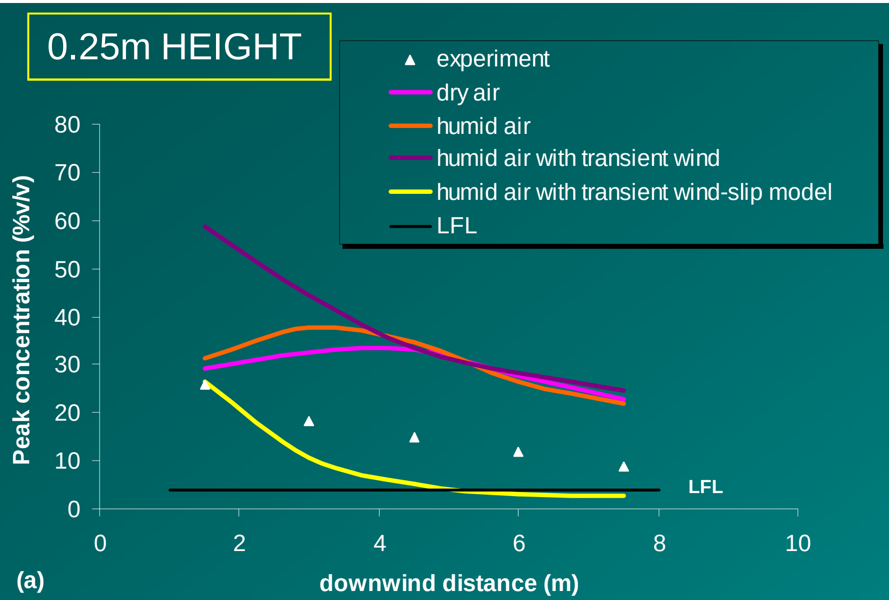


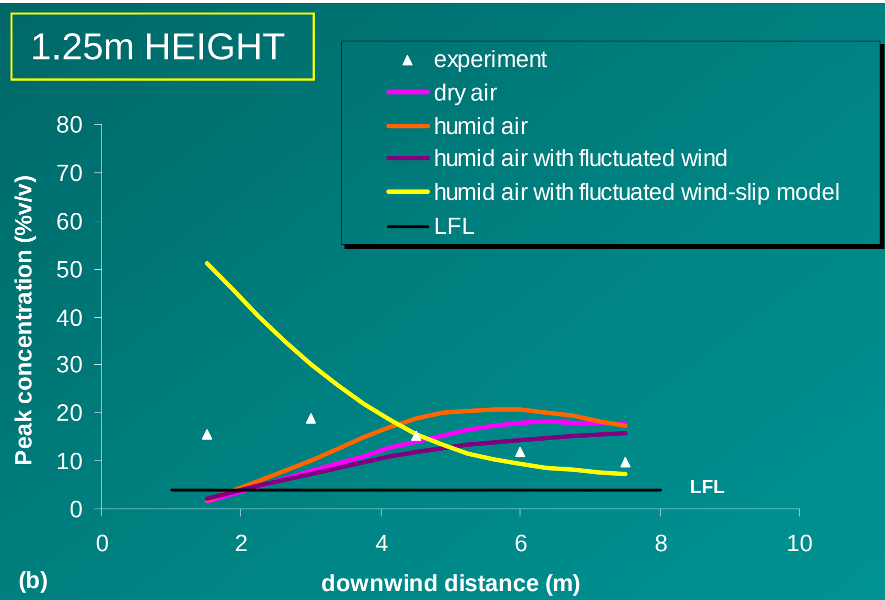

0.25m HEIGHT

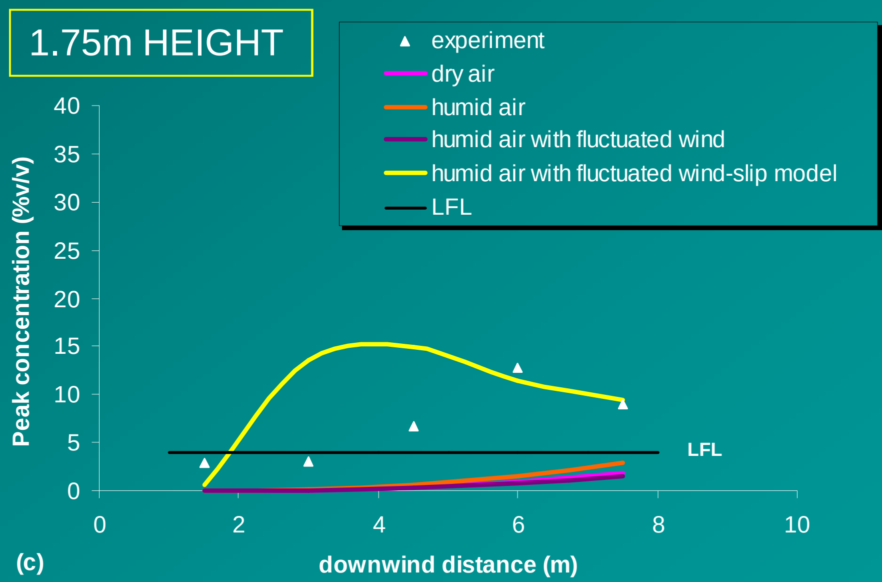
1.75m HEIGHT



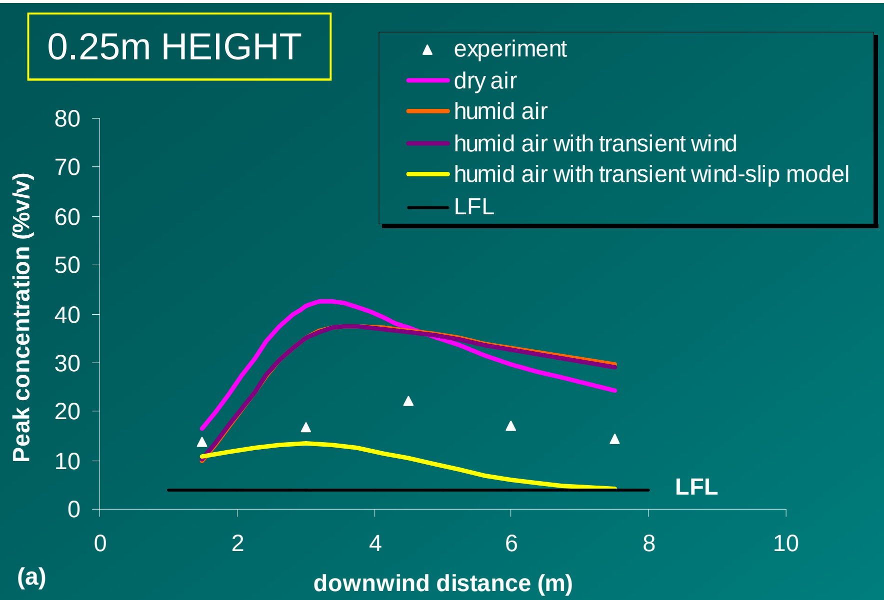
# RESULTS (TEST 6)

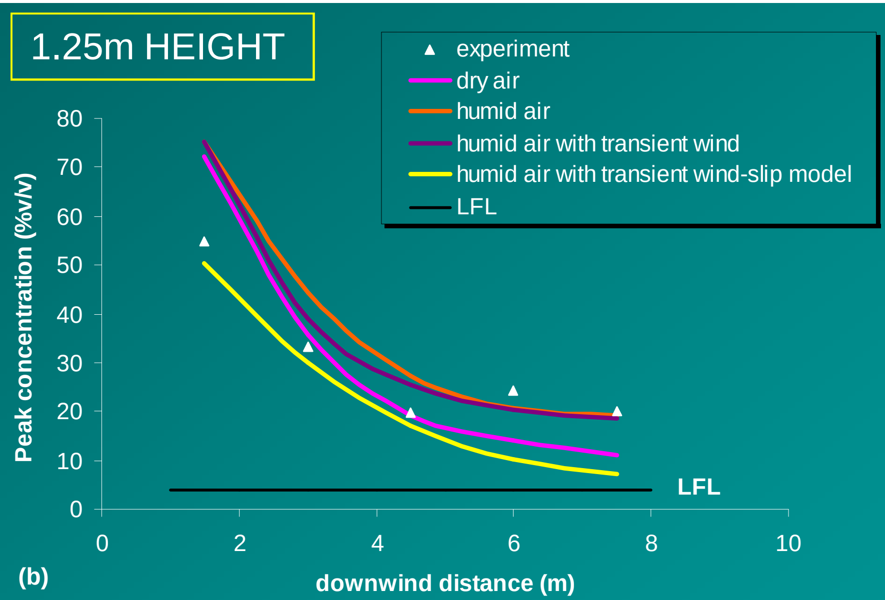


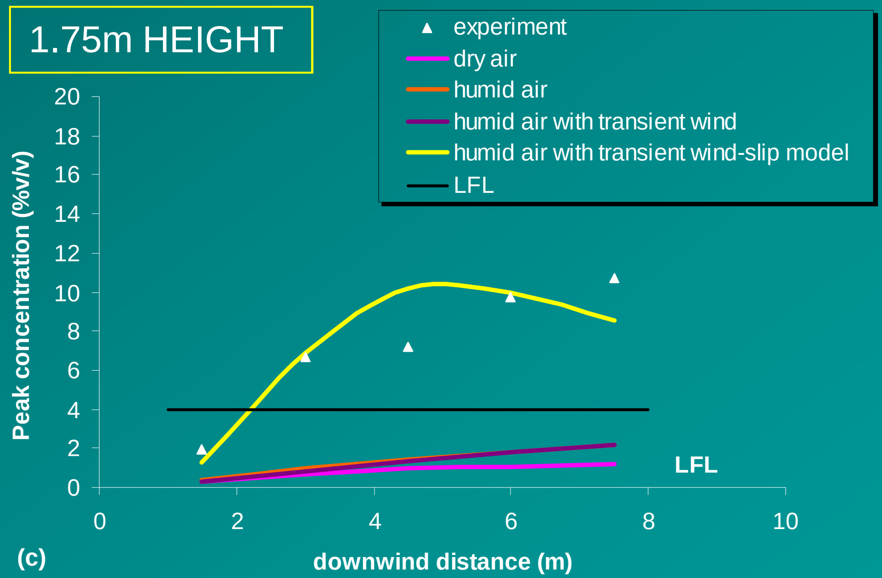



# RESULTS (TEST 7)




** Yellow line is with coarse grid*



# CONCLUSIONS

- LH2 dispersion in open environment was simulated using HSL experiments
- Ambient humidity, wind direction, and slip effect were examined
- Humidity affects the dispersion. It makes the cloud more buoyant.
- Slip effect should be considered in two phase releases, especially when humidity is solved, in order to “see” the buoyancy effect.
- High wind direction fluctuations during large time intervals influence the course of the cloud.
  - When the calculation of the safety area is important wind direction is also important.
  - However, comparison with the maximum H2 concentrations in line with the release provide valuable information.
- The best simulation case (humidity + slip effect + transient wind direction) for test 5 and 6 is consistent with the experiment.
- For test 7 the cases without slip terms give underestimation for the H2 concentration at the higher sensors. Slip model improved the computational results even though a coarser grid was used.

# FUTURE WORK

- Examination of slip effect in Test 7 with the fine grid.
- The air condensation ($N_2$ and $O_2$) and its effect on the prediction will be examined.
- Other slip models could be examined.
- Other wind profiles could be tested. A smoothing filter can be used.
- Heat flux from the ground to the cryogenic pool, using the boiling curve correlations will be implemented in ADREA-HF code and tested.

# ANY QUESTIONS

**THANK YOU FOR YOUR ATTENTION**