DEVELOPMENT AND APPLICATION OF THE MICROSCALE LAGRANGIAN PARTICLE DISPERSION MODEL MICROSPRAY FOR THE SIMULATION OF HYDROGEN ACCIDENTAL RELEASES

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Harmo 13, Paris, 1-4 June 2010

The framework: BioH2Power Project, WP5

Detailed modelling for a safe design of the unit

The main objective of WP5 is to study the reliability and safety issues during the realisation of innovative systems for the H2 production from biomass (the BioH2Power Unit).

This task is accomplished following two main research lines:

-) study and development of numerical models specifically aimed at simulating the dispersion of non-neutral (positively or negatively buoyant) gases as a tool for the safety analysis of H2 production from biogases

-) assessment of the reliability and safety of the system configurations under study, and identification of the actions to be performed to refine the system design.

WP 5 numerical modelling activity: **the rationale**

Development of a new version of the 3-D Lagrangian stochastic dispersion model MicroSpray (**μSPRAY**), which is regularly used for estimating the airborne pollutant dispersion, specially devoted to simulate accidental gaseous releases at the microscale.

Implementation of new modules, specifically tailored to treat the physics of accidental release and dispersion of non-neutral gases (*exit gas density higher or lower than that of the environmental air*) in the model, aimed at considering also particular conditions, such as high exit speed of the gas (*jets*).

The new model supports the safety study for the planning and building of the BioH2Power units.

WP 5 numerical modelling activity: **the strategy**

- Study and investigation of the phenomenology of the hydrogen release and dispersion

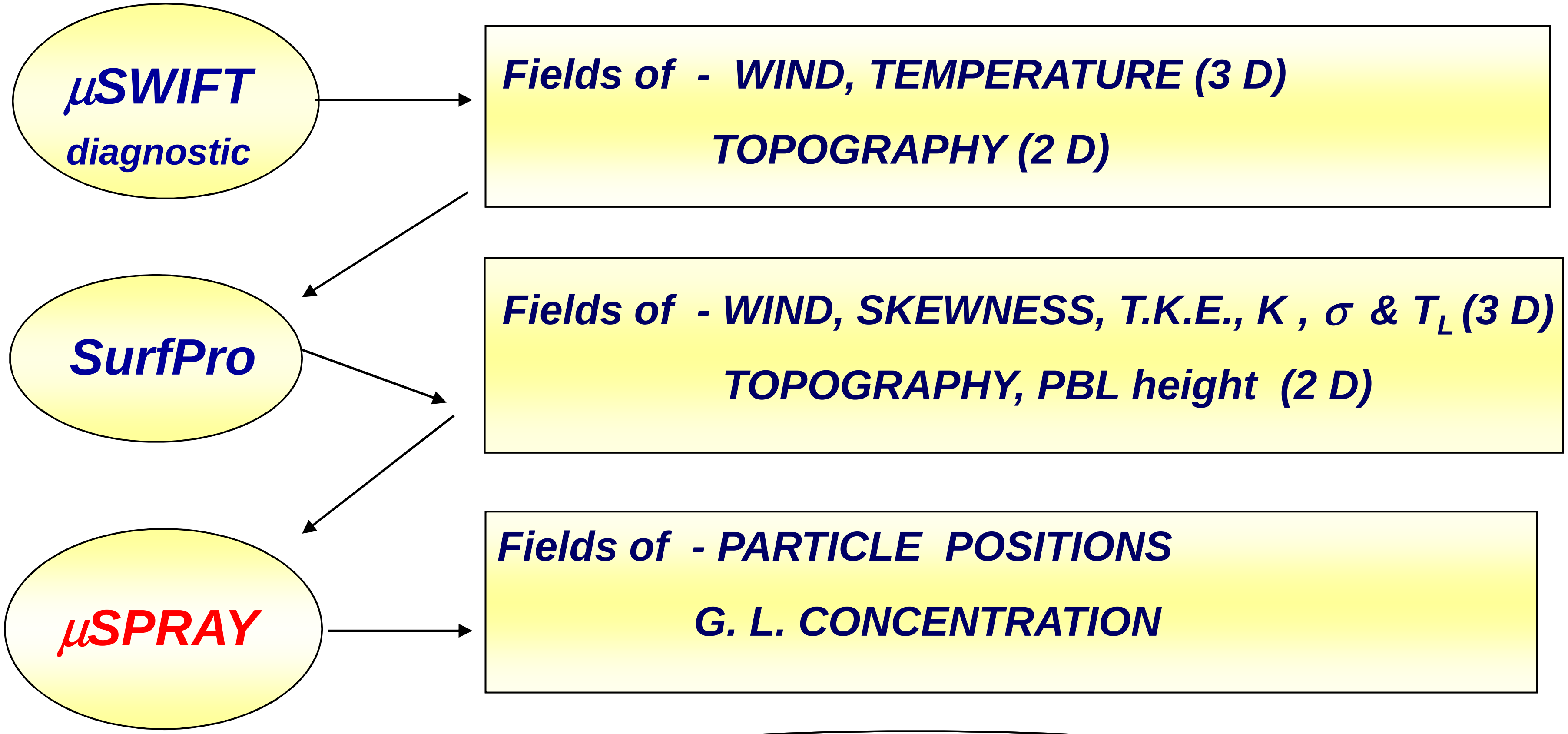
- Selection and numerical implementation of a mathematical model for light gas plume rise

- Analysis and selection of hydrogen release and dispersion experiments in literature and setup of a focused measuring campaign → Pisa experiment.

- Validation of the new plume rise module on experimental data

The MSS modelling system 1/2

ARIANET Milan, ARIA Paris, ISAC/CNR Turin



μSWIFT

diagnostic

Fields of - WIND, TEMPERATURE (3 D)

TOPOGRAPHY (2 D)

SurfPro

Fields of - WIND, SKEWNESS, T.K.E., K , σ & T_L (3 D)

TOPOGRAPHY, PBL height (2 D)

μSPRAY

Fields of - PARTICLE POSITIONS

G. L. CONCENTRATION

Obstacles & buildings included !

The MSS modelling system 2/2

… it allows taking into account:

- negatively, positively or neutral emissions in presence of obstacles
- any kind of source configuration, with emission in any direction and any initial velocity
- dispersion of dense and/or light gas, accidental releases and possible terrorist attacks in urban areas.

The MSS modelling system for light/dense gas 1/4

The idea beneath: to implement a plume rise model capable of treating buoyant plumes in complex atmospheric structure since it integrates along the plume trajectory.

An entrainment parameterisation to specify the mixing of ambient air into the plume is integrated into the differential equations for the fluid motion

REFERENCES:

Glendening, J.W., J.A. Businger, and R.J. Farber, (1984), "Improving plume rise prediction accuracy for stable atmospheres with complex vertical structure". ***J. Air Pollut. Control Ass.*****, 34 : 1128–1133**

Hurley, P.J., and P.C. Manins (1995) "Plume rise and enhanced dispersion in LADM.", ***CSIRO Division of Atmospheric Research*****, ECRU Technical Note No.4**

Hurley P.J. (2005) "The Air Pollution Model (TAPM) Version 3. Part1: Technical Description"***. CSIRO Atmospheric Research Technical Paper*** **No. 71**

The MSS modelling system for light/dense gas 2/4

The variables

$\vec{u}_p = (u_p, v_p, w_p) = u_s \vec{s}$	plume velocity vector in a cartesian reference system determined by $\vec{s}$, $\vec{n}$ axes
$\vec{u}_a = (u_a, v_a, w_a)$	wind velocity vector in the cartesian reference system
$u_e = u_e^{rise} + u_e^{turb}$	entrainment velocity
b	plume radius
ρ_p, T_p, ϑ_p	density, temperature and potential temperature of the gas
ρ_a, T_a, ϑ_a	density, temperature and potential temperature of the air
ϕ_p, ψ_p	angles between the plume direction $\vec{s}$ and the xz and xy planes
ϕ_a, ψ_a	angles between the airflow velocity $\vec{u}_a$ direction and the xz and xy planes

The MSS modelling system for light/dense gas 3/4

The equations 1/2

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}u_s\,b^2\right]= E\,u_s$$

mass conservation

$$\frac{d}{dt}\left[u_s\,b^2\,B\right]=-\frac{\rho_p}{\rho_a}N^2\,u_s\,w_p\,b^2$$

energy conservation

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}u_s\,w_p\,b^2\right]= Bb^2\,u_s$$

vertical momentum conservation

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}u_s\,b^2\,u_p\right]= E\,u_s\,u_a$$

X horizontal momenta conservation

$$\frac{d}{dt}\left[\frac{\rho_p}{\rho_a}u_s\,b^2\,v_p\right]= E\,u_s\,v_a$$

Y horizontal momentum conservation

The MSS modelling system for light/dense gas 4/4

The equations 2/2

Five unknowns $r_{\mathrm{p}}, u_p, v_p, w_p, b$ where:

$$N^2 = \frac{g}{\vartheta_a}\frac{\partial \vartheta_a}{\partial z} \qquad B = g\,\frac{\rho_e - \rho_a}{\rho_a} \qquad E = 2\,b\,u_e$$

entrainment

Calculation of entrainment velocity as: $u_e = \left[\alpha_1 u_s + \alpha_2 Ua\right]$

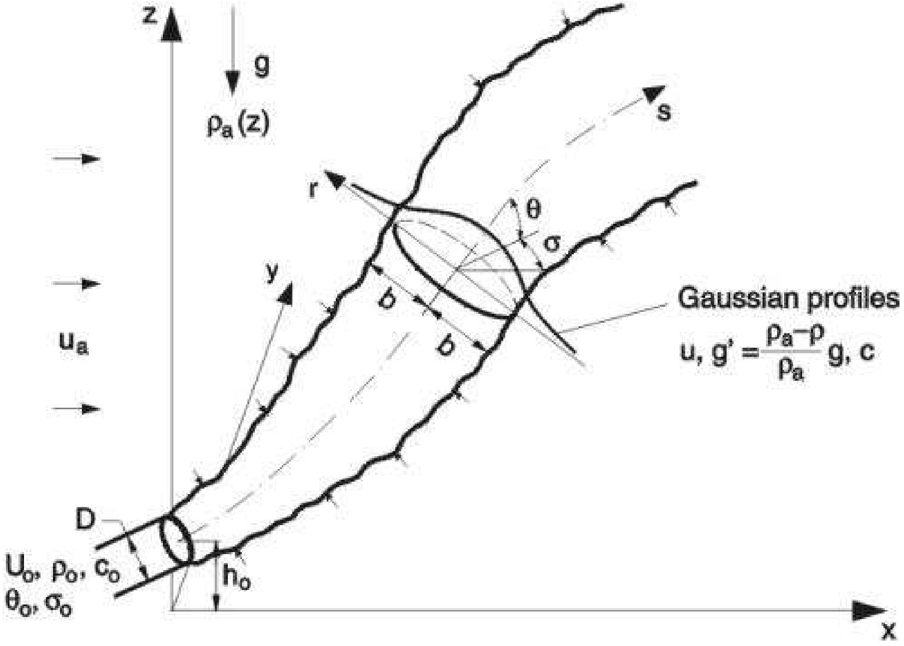
where

$$\begin{cases} |U_a| = \sqrt{u_a^{\,2} + v_a^{\,2} + w_a^{\,2}} \\ u_s = \sqrt{u_p^{\,2} + v_p^{\,2} + w_p^{\,2}} \end{cases}$$

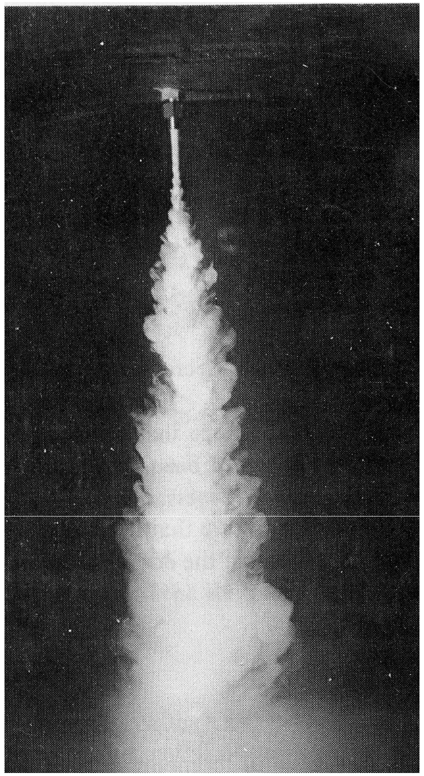
and $\alpha_1 = 0.1$ $\alpha_2 = 0.6$

Anfossi D., Tinarelli G., Trini Castelli S., Nibart M., Olry C., Commanay J., 2010. *A new Lagrangian particle model for the simulation of dense gas dispersion*. Atmospheric Environment, 44, 753-762

Expected dynamics of buoyant jet and plume

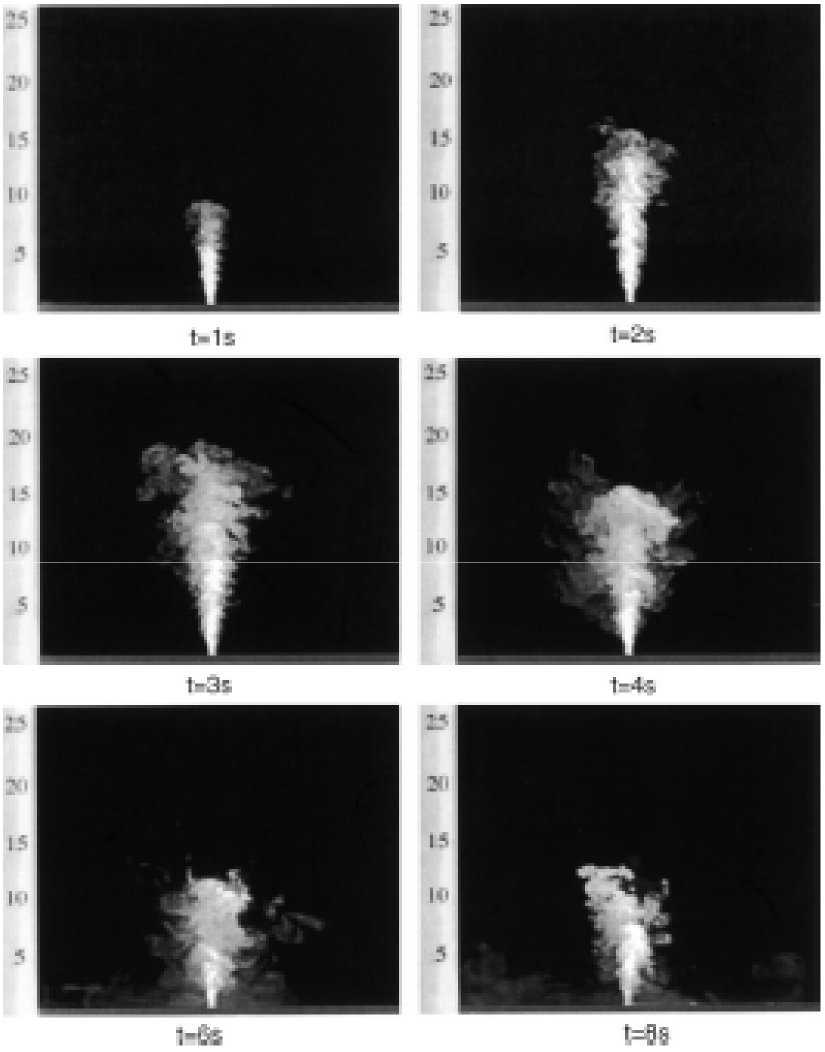


Buoyant plumes

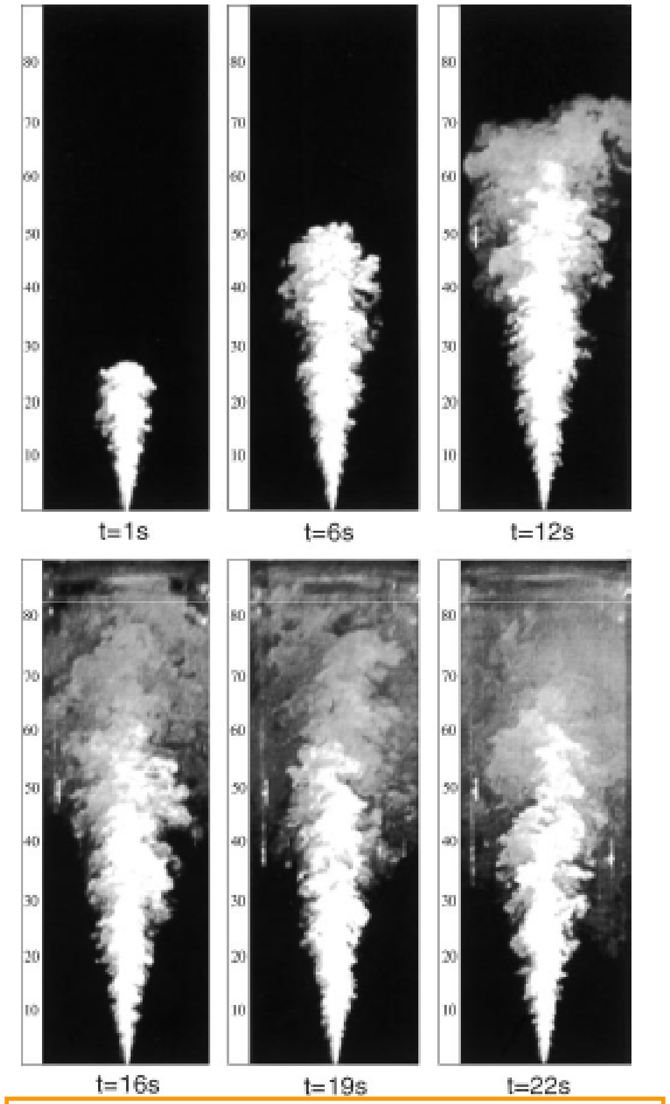


Jets. Buoyant fluid emerging from a nozzle into an otherwise undisturbed tank of water. *Scorer R.S., 1978.*

From: Pantzlaff and Lueptow, “Transient negatively and positively buoyant turbulent round jets”, Experiments in Fluids 27 (1999)



Negatively buoyant jet



Positively buoyant jet

The PISA experimental campaign

Analysis and selection of hydrogen release and dispersion experiments in literature and setup of a focused measuring campaign → … joining the Pisa experiment.

AIM: to gather specific experimental data of dispersion and concentrations in real atmosphere for typical H_2 accidental releases: high emission velocities, light gas →→

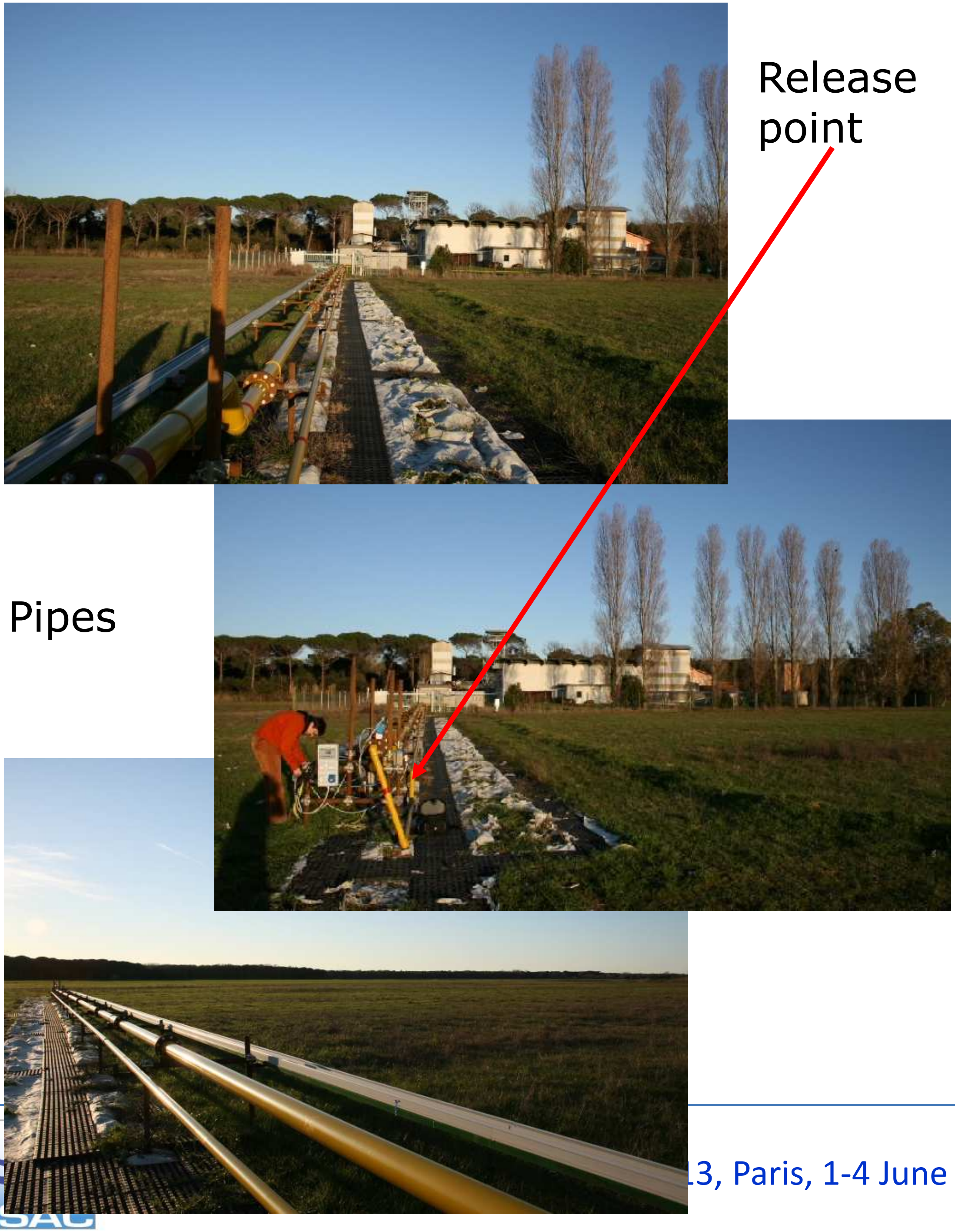
→ Verification of new modules in MicroSpray

→ Validation of MicroSpray simulations

Pisa experiment: in collaboration with Politecnico of Torino (Prof. A. Carpignano) and University of Pisa (Prof. M. Carcassi).

A sonic anemometer provided by ISPESL (Dr. A. Pelliccioni), Roma

Extreme microscale !

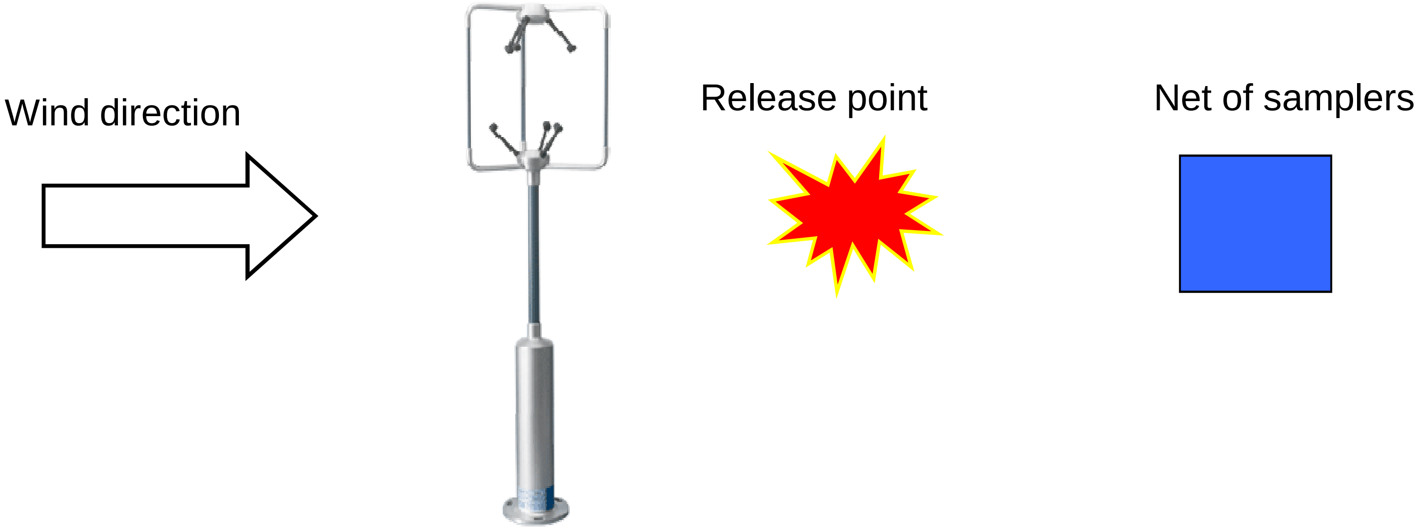


Release point

Pipes

Release equipment

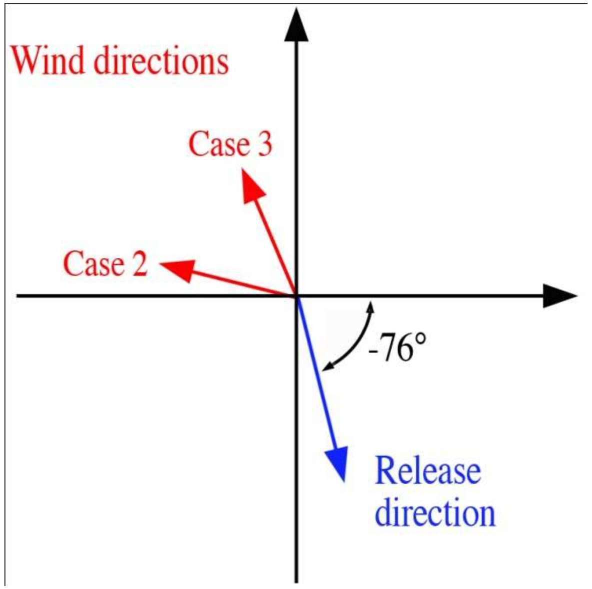
The PISA experimental campaign: design sketch

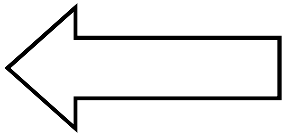


Wind direction

Release point

Net of samplers





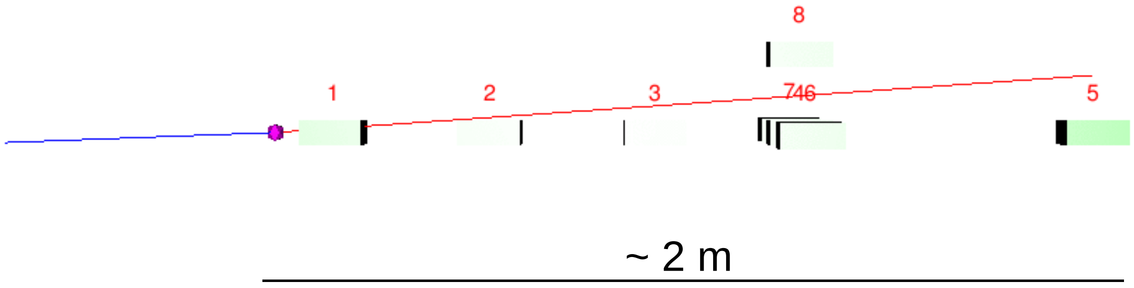
Wind direction

But in the real field…..

The PISA experimental campaign: design sketch

Sensor locations

Case 2



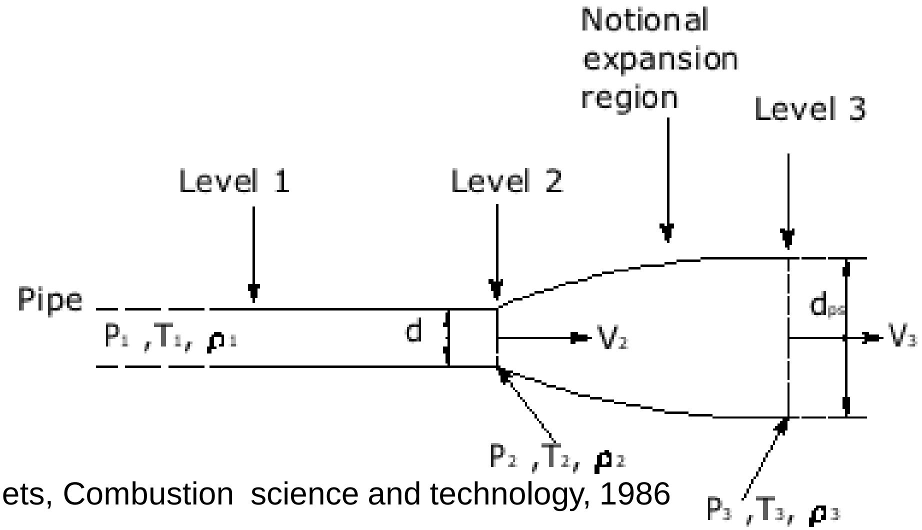
Release	wind direction	wind speed	Friction velocity u_*	Roughness z_0	St. Dev. σ_u	St. Dev. σ_v	St. Dev. σ_w
1	98	1.00	0.10	0.018	0.25	0.24	0.07
2	**114**	**0.96**	**0.13**	**0.052**	**0.30**	**0.57**	**0.11**
3	157	1.61	0.10	0.0016	0.66	0.29	0.09

The PISA experimental campaign: the source

$T_1 = 298\ K$

$d = 11\ mm$

$S = 9.5 \cdot 10^{-5}\ m^2$



Birch et al., Velocity decay of high pressure jets, Combustion science and technology, 1986

$$P_1 = 10 \cdot 10^5\ Pa$$

$$\rho_1 = \frac{P_1}{R_{H_2} T_1} = 0.813\ Kg/m^3$$

$$\dot{m} = S\sqrt{P_1 \rho_1} \cdot 0.686 = 0.059\ Kg/s$$

$$V_3 = V_2 \left\{ C_D + \frac{1 - \frac{P_a}{P_1}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{1-\gamma}}}{\gamma C_D} \right\} = 1982\ m/s$$

$$d_3 = d_{ps} = d\, C_D \sqrt{\frac{P_1}{P_a}\left(\frac{2}{\gamma-1}\right)^{\frac{1}{\gamma-1}} \frac{\gamma}{\gamma C_D^2 + 1}} = 0.019\ m$$

$$P_1 = 7 \cdot 10^5\ Pa$$

$$\rho_1 = \frac{P_1}{R_{H_2} T_1} = 0.569\ Kg/m^3$$

$$\dot{m} = S\sqrt{P_1 \rho_1} \cdot 0.686 = 0.041\ Kg/s$$

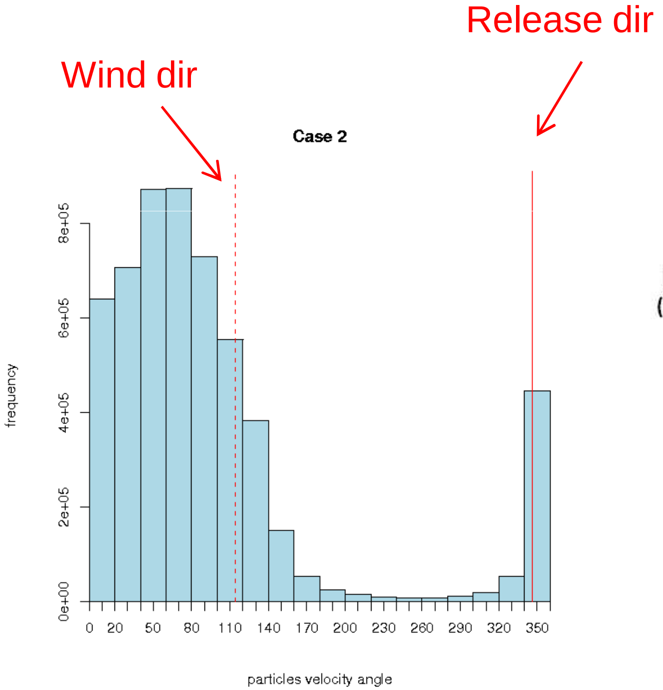
$$V_3 = V_2 \left\{ C_D + \frac{1 - \frac{P_a}{P_1}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{1-\gamma}}}{\gamma C_D} \right\} = 1888\ m/s$$

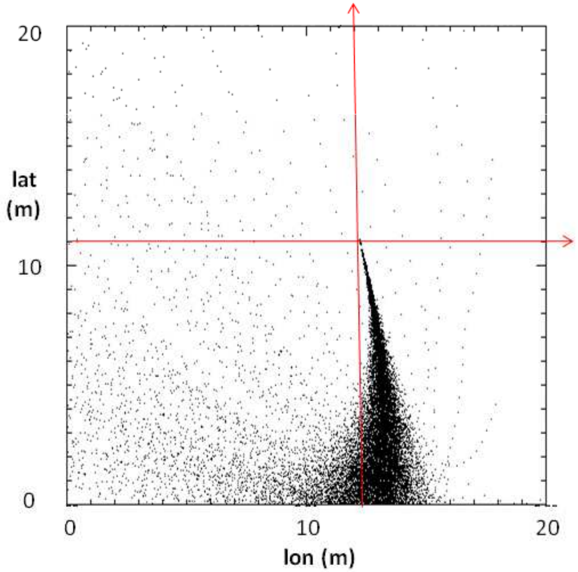
$$d_3 = d_{ps} = d\, C_D \sqrt{\frac{P_1}{P_a}\left(\frac{2}{\gamma+1}\right)^{\frac{1}{\gamma-1}} \frac{\gamma}{\gamma C_D^2 + 1}} = 0.016\ m$$

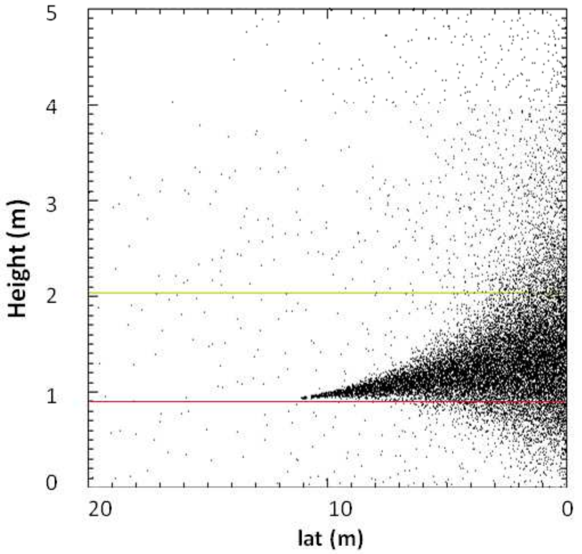
The PISA MSS numerical simulations:
velocity distribution and plume dynamics

Case 2 ← **Example here**

The experiments and the numerical simulations last approximately 80s
The concentrations are calculated in the last 20s







The PISA MSS numerical simulations: concentration

…where Δx, Δy, Δz is the 'concentration grid'

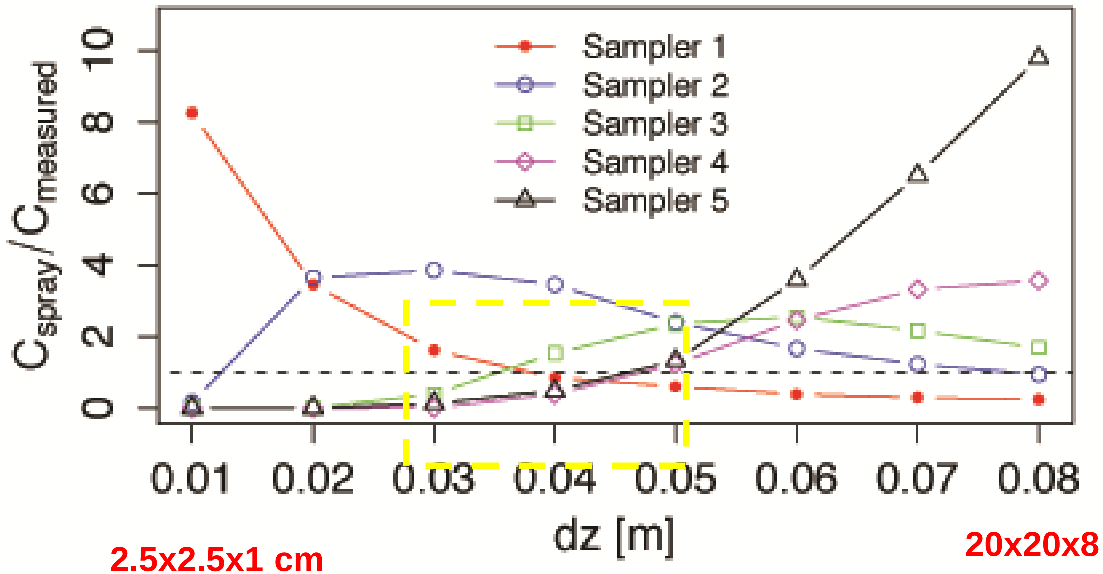
$$C(i,j,k)=\frac{M(i,j,k)}{\Delta x\Delta y\Delta z}$$

Counting the number of particles in each grid cell and accumulating their masses

$$C(i,j,k)=\frac{M(i,j,k)}{\Delta x\Delta y\Delta z}\boxed{\frac{U_p\Delta t}{\Delta x}}$$

The contribution of each particle mass is weighted by the total time the particle spends inside the cell during its time step

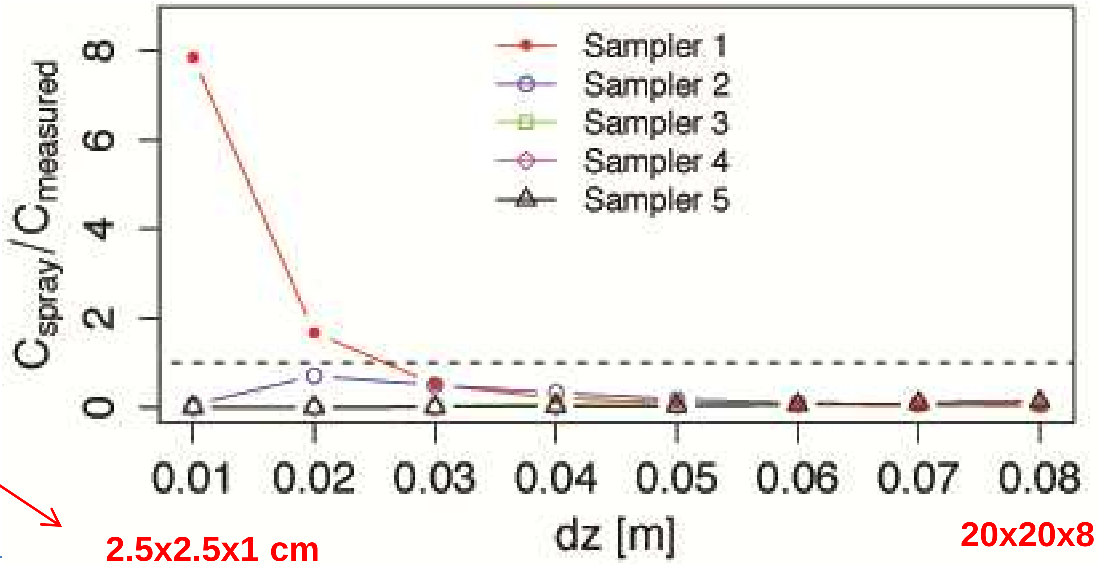
The PISA MSS numerical simulations: concentration



2.5x2.5x1 cm

20x20x8 cm

Dimension of the sampling box of calculated concentrations



2.5x2.5x1 cm

20x20x8 cm

Present progress in the study…..

-) study and development of numerical models specifically aimed at simulating the dispersion of non-neutral (positively or negatively buoyant) gases as a tool for the safety analysis of H2 production from biogases

-) further analysis of the new plume rise numerical modules and of the Pisa experiment results

1. Some sensitivity analysis on the experiment configuration
2. Investigation of new algorithms for supersonic speed emission: jets
3. Investigation of new algorithms for unintended hydrogen releases

Investigation of new algorithms for supersonic speed emission: jets

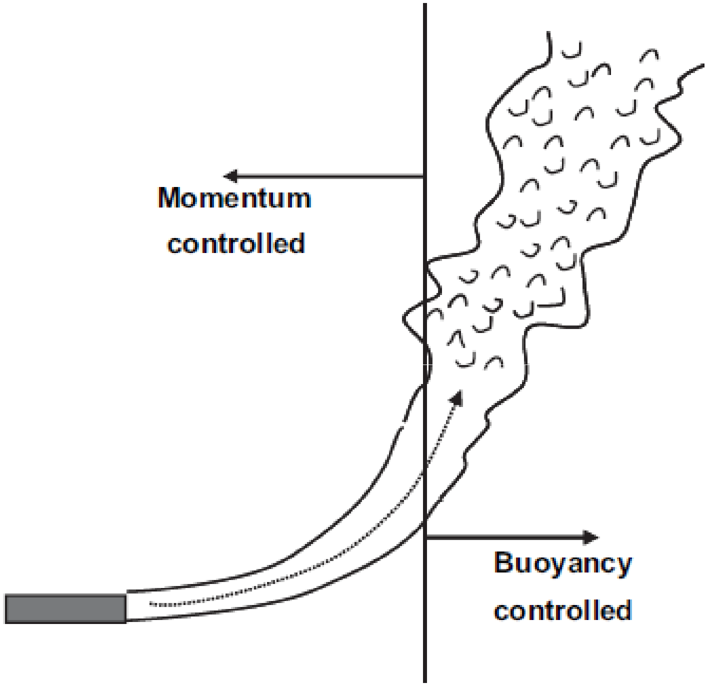


Fig. 1. Schematics diagram of buoyant jet dispersion.

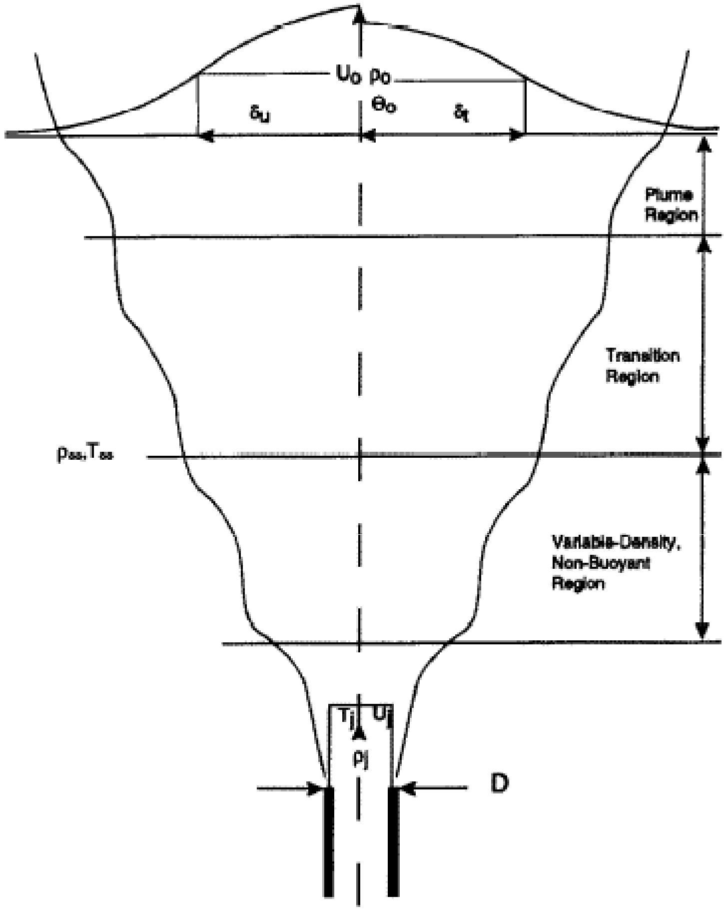


FIG. 1. The three different regions of a buoyant jet.

Plume region

Transition region

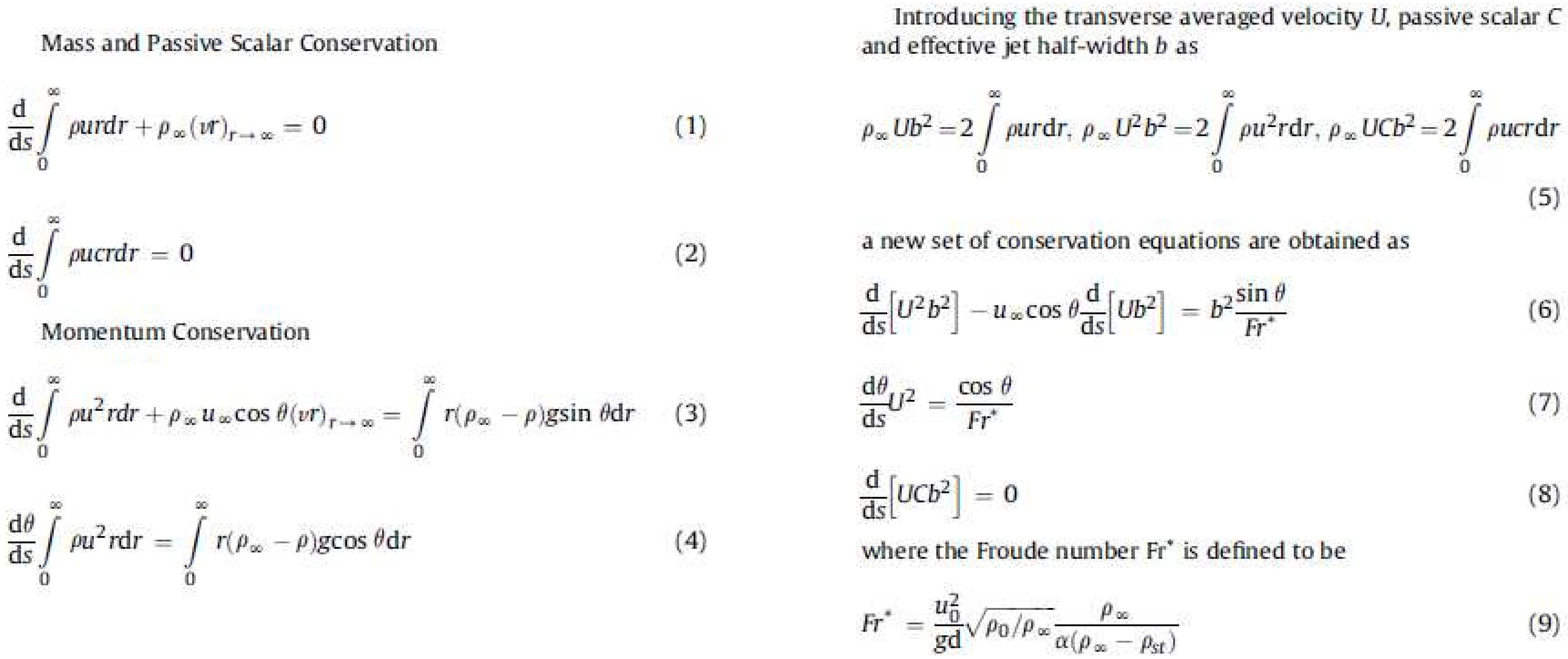
Variable-density non-buoyant region

Kim J.S., W. Yang, Y. Kim, S.H., Won,W., 2010.
J. of Loss Prevention in the Process Industries

So and Aksoy, 1993,
Int. J. Heat Mass Transfer 36, 3187-3200

Investigation of new algorithms for supersonic speed emission: jets

Kim J.S., W. Yang, Y. Kim, S.H., Won,W., 2010. Behavior of buoyancy and momentum controlled hydrogen jets and flames emitted into the quiescent atmosphere. Journal of Loss Prevention in the Process Industries



Mass and Passive Scalar Conservation

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_0^\infty \rho u r \mathrm{d}r + \rho_\infty (vr)_{r\to\infty} = 0 \quad (1)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_0^\infty \rho u c r \mathrm{d}r = 0 \quad (2)$$

Momentum Conservation

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_0^\infty \rho u^2 r \mathrm{d}r + \rho_\infty u_\infty \cos\theta (vr)_{r\to\infty} = \int_0^\infty r(\rho_\infty - \rho) g \sin\theta \mathrm{d}r \quad (3)$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}s}\int_0^\infty \rho u^2 r \mathrm{d}r = \int_0^\infty r(\rho_\infty - \rho) g \cos\theta \mathrm{d}r \quad (4)$$

Introducing the transverse averaged velocity U, passive scalar C and effective jet half-width b as

$$\rho_\infty U b^2 = 2\int_0^\infty \rho u r \mathrm{d}r,\ \rho_\infty U^2 b^2 = 2\int_0^\infty \rho u^2 r \mathrm{d}r,\ \rho_\infty U C b^2 = 2\int_0^\infty \rho u c r \mathrm{d}r \quad (5)$$

a new set of conservation equations are obtained as

$$\frac{\mathrm{d}}{\mathrm{d}s}\left[U^2 b^2\right] - u_\infty \cos\theta \frac{\mathrm{d}}{\mathrm{d}s}\left[U b^2\right] = b^2 \frac{\sin\theta}{Fr^*} \quad (6)$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}s} U^2 = \frac{\cos\theta}{Fr^*} \quad (7)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\left[U C b^2\right] = 0 \quad (8)$$

where the Froude number Fr^* is defined to be

$$Fr^* = \frac{u_0^2}{gd}\sqrt{\rho_0/\rho_\infty}\frac{\rho_\infty}{\alpha(\rho_\infty - \rho_{st})} \quad (9)$$

Investigation of new algorithms for supersonic unintended hydrogen releases

W. Houf, R. Schefer, 2008. Analytical and experimental investigation of small-scale unintended releases of hydrogen. International Journal of Hydrogen Energy, 33, 1435-1444

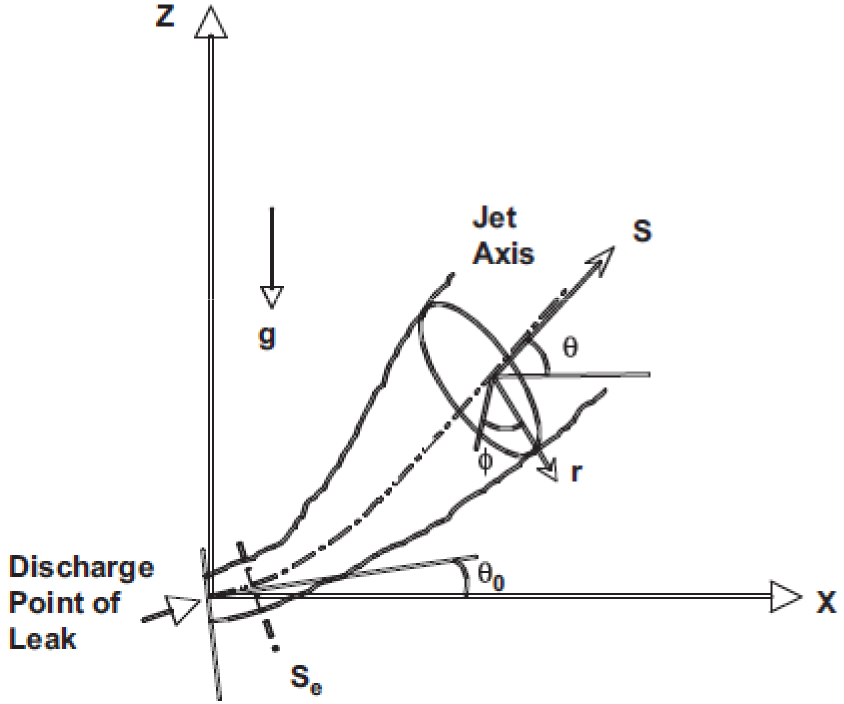


Fig. 2 – Schematic of hydrogen slow leak buoyant jet model.

$$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho u r\,dr\,d\phi = \rho_{\infty}E \qquad (2)$$

$$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho u^2\cos\theta r\,dr\,d\phi = 0 \qquad (3)$$

$$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho u^2\sin\theta r\,dr\,d\phi = \int_0^{2\pi}\int_0^{\infty}(\rho_{\infty}-\rho)gr\,dr\,d\phi \qquad (4)$$

$$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho u(y-y_{\infty})r\,dr\,d\phi = 0 \qquad (5)$$

$$\frac{\partial}{\partial S}(X) = \cos\theta \qquad (6)$$

$$\frac{\partial}{\partial S}(Z) = \sin\theta \qquad (7)$$

Investigation of new algorithms for supersonic speed emission: unintended hydrogen releases

W. Houf, R. Schefer, 2008. Analytical and experimental investigation of small-scale unintended releases of hydrogen. International Journal of Hydrogen Energy, 33, 1435-1444

As the jet exits the leak the turbulent mixing layers at the edges of the jet begin to grow and eventually expand to merge at the centerline of the jet.

$$u(S,r,\phi) = u_{cl}(S)\exp[-r^2/b^2] \tag{8}$$

$$\rho(S,r,\phi) = \rho_\infty - (\rho_\infty - \rho_{cl}(S))\exp[-r^2/\lambda^2 b^2] \tag{9}$$

$$\rho(S,r,\phi)y(S,r,\phi) = \rho_{cl}(S)y_{cl}(S)\exp[-r^2/\lambda^2 b^2] \tag{10}$$

$$E = E_{mom} + E_{buoy} \tag{11}$$

$$E_{mom} = 0.282\left(\frac{\pi D^2}{4}\frac{\rho_{exit}U_{exit}^2}{\rho_\infty}\right)^{1/2} \tag{12}$$

$$E_{buoy} = \frac{a_2}{Fr_l}(2\pi U_{cl}b)\sin\theta \tag{13}$$

$$Fr_l = \frac{U_{cl}^2}{(gD(\rho_\infty - \rho_{cl})/\rho_{exit})} \tag{14}$$

Conclusion and work in process

The numerical simulation of the Pisa experimental trials show that the non-neutral version of µSPRAY is able to simulate such peculiar and extreme condition:
also with a supersonic jet of a buoyant gas in a very small environment, the model is able to reproduce the particles' motion and to give a reasonable concentration estimation.

Nevertheless the interpretation of µSPRAY results has to be coupled to the interpretation of the experimental measurements.
In fact, during the data analysis and the numerical simulations a lot of issues arose:

- *an uncertainty in the emission angle with respect to the anemometer position;*
- *a strong fluctuations of the sensor position;*
- *a crucial dependence of the particles' dispersion on the initial conditions (related to the small scale and the velocity of the release).*

Under process for next improvement……

- further simulations varying the initial and boundary conditions in the model, on the basis of the experimental uncertainties;
- sensitivity analysis on the turbulence variables;
- **new specific formulations and algorithm were analyzed for supersonic release speeds (jets) and unintended hydrogen leaks.**