HIGHLY RESOLVED LARGE EDDY SIMULATIONS OF A LAMINAR-TURBULENT TRANSITIONAL AIR-HELIUM BUOYANT JET IN A TWO VENTED ENCLOSURE: VALIDATION AGAINST PARTICLE IMAGE VELOCIMETRY EXPERIMENTS

E. SAIKALI$^{1,2,3}$  G. BERNARD-MICHEL$^1$  A. SERGENT$^{2,4}$  C. TENAUD$^2$

$^1$CEA Saclay - DEN/DANS/DM2S/STMF/LIEFT, 91191 Gif-sur-Yvette cedex, France
$^2$LIMSI-CNRS (ETCM), Université Paris-Saclay, 91405 Orsay, France
$^3$IFD, ED391 SMAER, UPMC Paris 06, Sorbonne Universités, 75006 Paris, France
$^4$UFR 919 Ingénierie, UPMC Paris 06, Sorbonne Universités, 75005 Paris, France

International Conference on Hydrogen Safety (ICHS 2017)
September 12, 2017 – Hamburg (Germany)
Hydrogen Safety: 
Non-nuclear applications
Model: physical set-up

- Fuel cell, garage ⇒ Parallelepiped cavity,
- Hydrogen leakage ⇒ Injection of helium $\rho_{\text{amb}}/\rho_{\text{inj}} = 7.24$ at $25^\circ$ C (real ratio to hydrogen is 14.38) [Bernard-Michel and Houssin-Agbomson, 2017],
- Reducing the mixture concentration ⇒ Vented cavity,
- Laminar-turbulence transition ⇒ OK [Chen and Rodi, 1980],
- Jet spreading ⇒ OK [Kalter et al., 2014].
- Iso-thermal ans iso-bar conditions: $p = 10^5$ Pa and $T = 298.15$ K.
Methodology and key points

Approaches
- Experiment, PIV measurements,
- Numerical approach (currently LES), PIV validation.

Interest
- Buoyant jet regime ($Q = 5 \text{ Nl/min}, \text{Ri}_{inj} = 0.14$ ),
- Homogeneous layer with stratification ($\text{Ri}_v = 0.99$),
- Limited domain, two vents, BC issue.

Main issues
- CFD code challenge (high gradients, rapid laminar-turbulent transition),
- Outlet boundary condition treatment, two outlet challenge,
- Predictive models (free/limited media),
- No similar work reported in the literature.
LES formulation (LMN approximation)

> Low Mach Number (LMN) hypothesis ⇒ Pressure = \( p(t) + P(x, t) \) [Müller and Muller, 1999]

\[
\begin{align*}
\frac{\partial \bar{\rho} \tilde{Y}_1}{\partial t} &+ \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i \tilde{Y}_1) = \frac{\partial \tilde{\xi}_i}{\partial x_i} + \frac{\partial \tilde{\xi}_i^{SGS}}{\partial x_i}, \\
\bar{\rho} &\equiv \frac{p M}{R T}, \\
\frac{\partial \bar{\rho} \tilde{u}_j}{\partial t} &+ \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_j \tilde{u}_i) = - \frac{\partial \bar{P}}{\partial x_j} + \frac{\partial \tilde{P}}{\partial x_i} + \frac{\partial \tilde{\tau}_{ij}^{SGS}}{\partial x_i} + \bar{\rho} g_j, \\
\frac{\partial \bar{\rho}}{\partial t} &+ \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i) = 0,
\end{align*}
\]

where \( \tilde{\cdot} \) the spatial filter symbol, \( \bar{\varphi} = \bar{\rho} \varphi / \bar{\rho} \) (Favre), \( \bar{u} = (\bar{u}_1, \bar{u}_2, \bar{u}_3) \), \( \tilde{\xi}_i = \bar{\rho} D \frac{\partial \bar{Y}_1}{\partial x_i} \), \( D = 6.91 \times 10^{-5} \)

\( m^2.s^{-1} \), \( \bar{M} = (\sum_{i=1}^{2} \frac{\bar{Y}_i}{\bar{M}_i})^{-1} \), \( \tilde{\tau}_{ij} = 2 \mu \bar{e}_{ij} \) with \( \bar{e}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{1}{2} \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} \) and \( \bar{g}_j = (0, 0, -g) \).

> Additional SGS terms closed as

\[
\tilde{\tau}_{ij}^{SGS} = \bar{\rho} (\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j) = 2 \mu_{SGS} \bar{e}_{ij} \quad \text{and} \quad \tilde{\xi}_i^{SGS} = \bar{\rho} (\bar{u}_i \bar{Y}_1 - \bar{u}_i \bar{Y}_1) = \frac{\mu_{SGS}}{S_{SGS}} \frac{\partial \bar{Y}_1}{\partial x_i},
\]

where \( \mu_{SGS} = \bar{\rho} (C_s \Delta)^2 \sqrt{2 \bar{e}_{ij} \bar{e}_{ij}}, \Delta = (\delta_x \delta_y \delta_z)^{1/3}, \ C_s = 0.18 \) and \( S_{SGS} = 0.7 \) [Blanquart and Pitsch, 2008].

Remark

Average symbols \( \bar{\cdot} \) and \( \tilde{\cdot} \) are removed for simplicity in the sequel.

E. Saikali
ICHIS 2017
Tuesday 12 September, 2017 5 / 20
Numerical methods & Boundary conditions

- Semi-implicit scheme (diffusion implicitly), CFL\textsubscript{conv},
- Finite difference volume on staggered grid,
- Spatial discretization: 2nd order center (NS-equation), 3rd order QUICK (species) for $Y_1 \in [0, 1]$,
- Temporal discretization: 2nd order Runge-Kutta,
- Pressure-velocity incremental projection method (Poisson equation).

- IC’s : Cavity filled with pure ambient at rest ($u = 0, Y_1 = 0$),

- BC’s : \( \partial \Omega = \partial \Omega_w \cup \partial \Omega_i \cup \partial \Omega_o \),
  - \textit{Wall boundaries} (\( \partial \Omega_w \)). No slip \( u = 0, \frac{\partial \varphi}{\partial (x \cdot n)} = 0 \) : \( \varphi = \{ P, \rho, Y_1 \} \).
  - \textit{Injection boundary} (\( \partial \Omega_i \)). Constant injection mass flux \( \rho_{inj} Q \), Poiseuille \( u \) profile, \( \rho = \rho_{inj}, Y_1 = 1 \).
  - \textit{Outlet boundaries} (\( \partial \Omega_o \)). Ambient-equilibrium hydrostatic pressure \( P = -\rho_{amb} g z, \frac{\partial u}{\partial (x \cdot n)} = 0 \).

  If \( u \cdot n \geq 0 \), then \( \frac{\partial \varphi}{\partial (x \cdot n)} = 0 \) : \( \varphi = \{ \rho, Y_1 \} \).

  Else, \( Y_1 = 0 \) and \( \rho = \rho_{amb} \).

[CEA TRUST-TrioCFD, 2017]
Geometrical configurations

<table>
<thead>
<tr>
<th>Configuration</th>
<th>$L_x$ [cm]</th>
<th>Cell numbers</th>
<th>MPI procs</th>
</tr>
</thead>
<tbody>
<tr>
<td>0_x</td>
<td>2</td>
<td>1,134,404</td>
<td>20</td>
</tr>
<tr>
<td>1_x</td>
<td>3</td>
<td>2,129,220</td>
<td>40</td>
</tr>
<tr>
<td>2_x</td>
<td>3.5</td>
<td>2,609,476</td>
<td>40</td>
</tr>
<tr>
<td>3_x</td>
<td>4.5</td>
<td>3,329,860</td>
<td>60</td>
</tr>
<tr>
<td>4_x</td>
<td>6.75</td>
<td>4,427,588</td>
<td>80</td>
</tr>
<tr>
<td>5_x</td>
<td>10.125</td>
<td>6,108,484</td>
<td>100</td>
</tr>
</tbody>
</table>

- $\partial \Omega_W$ on red surfaces, $\partial \Omega_i$ on yellow surface and $\partial \Omega_o$ on blue surfaces.

- Unstructured uniform cubic mesh (per block) with cell size $\delta \approx 7 \times 10^{-4}$ m ($\delta / \eta = 3.3$ [Chhabra et al., 2006] where $\eta$ denotes the Kolmogorov length scale),

- 0.5 mm layer around the vents considered as $\partial \Omega_W$ (representing plexi-glass),

- Pipe $d = 1$ cm, $h = 10$ cm, Poiseuille velocity profile (entrance), $L_y = L_z = 2$ cm.
physical time of 110 seconds, statistics [70:110] s,
Velocity magnitude: vertical mid $xz$-plane
physical time of 110 seconds, statistics [70:110] s,

Velocity magnitude: vertical mid $xz$-plane

RMS (velocity magnitude): vertical mid $xz$-plane
Global quantities and convergence

> Integrated quantities

<table>
<thead>
<tr>
<th>Configurations</th>
<th>$&lt; M_{He} &gt; t \times 10^{-6}$ kg</th>
<th>$&lt; Q_{v}^{bot} &gt; t \times 10^{-4}$ m$^3$.s$^{-1}$</th>
<th>$&lt; Q_{v}^{top} &gt; t \times 10^{-4}$ m$^3$.s$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0_x$</td>
<td>8.98677</td>
<td>-2.5817</td>
<td>3.48674</td>
</tr>
<tr>
<td>$1_x$</td>
<td>8.10638</td>
<td>-2.81147</td>
<td>3.71449</td>
</tr>
<tr>
<td>$2_x$</td>
<td>8.30408</td>
<td>-2.80676</td>
<td>3.70839</td>
</tr>
<tr>
<td>$3_x$</td>
<td>8.20663</td>
<td>-2.77233</td>
<td>3.67504</td>
</tr>
<tr>
<td>$4_x$</td>
<td>8.47855</td>
<td>-2.60348</td>
<td>3.49892</td>
</tr>
<tr>
<td>$5_x$</td>
<td>8.45375</td>
<td>-2.60436</td>
<td>3.50027</td>
</tr>
</tbody>
</table>

where $M_{He} = \int_{V} \rho_{He} X_1 dV$ denotes the mass of He in the cavity of volume $V$, $X_1 = \rho Y_1 / \rho_{He}$ the helium volume fraction. The volumetric flow-rates $Q_{v}^{\Lambda} = \int_{\partial \Omega_{out}^{\Lambda}} u_1 d\sigma$, where $\Lambda = \{ \text{bot, top} \}$ and $\partial \Omega_{out}^{\text{bot}}, \partial \Omega_{out}^{\text{top}}$ denote the surface area of the bottom and top vent respectively.

> L2 norm relative error (conf $5_x$ is a reference)
Upper part of the cavity

- Lower cavity flow pattern: vertical mid \(xz\)-plane,

![Diagram showing flow patterns and velocity profiles](image)
Upper part of the cavity

- Lower cavity flow pattern: vertical mid $xz$-plane,

- Vertical $yz$-plane ($x = 2.95 \text{ cm}$) at the top vent surface: $< u_1 >_t \times$-horizontal velocity
CFD-PIV comparison

Conf 4_x

CFD

PIV

<table>
<thead>
<tr>
<th>x [cm]</th>
<th>0</th>
<th>2</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>y [cm]</td>
<td>0</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>z [cm]</td>
<td>0</td>
<td>2</td>
<td>4</td>
</tr>
</tbody>
</table>

z = 2 cm

z = 3.5 cm

z = 4.5 cm

z = 5.5 cm

z = 7 cm

z = 14 cm

E. Saikali

ICHS 2017

Tuesday 12 September, 2017 11 / 20
CFD-PIV comparison

The image displays a comparison between CFD ( Computational Fluid Dynamics) and PIV ( Particle Image Velocimetry) results. The graphs show velocity profiles at different vertical positions (z) as indicated on the left side of the image:

- z = 2 cm
- z = 3.5 cm
- z = 4.5 cm
- z = 5.5 cm
- z = 7 cm
- z = 14 cm

The graphs on the right side illustrate the comparison, with red lines representing CFD data and black circles representing PIV data. The x-axis represents the horizontal distance (cm), and the y-axis shows the velocity magnitude (m/s). The color scale on the top left indicates the range of velocity values.

The diagram also includes a 3D perspective view of the flow field, indicating the z-axis and the x-y plane with a red and blue color scheme to highlight different regions of interest.
- Two distinct behaviors, small/higher concentrations, E and axis take the highest above $z \approx 6.2$ cm,
- max concentration at top matches well (29%), thicker layer predicted,
- Geometry dependent, entrainment/mixing process, jet bending effect . . .

[Bernard-Michel et al., 2017, Hunt and Linden, 1999, Saikali et al., 2017a]
LES resolution
Concluding remarks and discussion

Main conclusion

- Flow analysis: helium distribution, air entrainment, recirculating zones, . . .
- Influence of the outlet boundary condition: similarities and discrepancies,
- Convergence on the size of the exterior domain,
  - Modification of the helium distribution depending the domain size,
  - PIV validation,
- Max concentration predicted by theoretical model, but flow is not divided through a two-layer stratification (Hunt-Linden framework).

Work to be continued (in progress)
- Global validation with new PIV data covering all domain,
- DNS computation ($\eta = 1.75 \times 10^{-4}$ m, $\approx 120 \times 10^6$ cells, 1988 MPI procs) for turbulence analysis: from turbulence fluxes and TKE budget to Boussinesq hypothesis validation,

Perspectives
- Development of boundary conditions able to mimic the presence of an exterior domain,
- Increasing the cavity's height and/or increasing/decreasing the injection flow-rate in the objective to produce a two-layer stratification,
- Hydrogen-air cases.
Concluding remarks and discussion

Main conclusion

- Flow analysis: helium distribution, air entrainment, recirculating zones, . . .
- Influence of the outlet boundary condition: similarities and discrepancies,
- Convergence on the size of the exterior domain,
  - Modification of the helium distribution depending the domain size,
  - PIV validation,
- Max concentration predicted by theoretical model, but flow is not divided through a two-layer stratification (Hunt-Linden framework).

Work to be continued (in progress)

- Global validation with new PIV data covering all domain,
- DNS computation ($\eta = 1.75 \times 10^{-4}$ m, $\approx 120 \times 10^6$ cells, 1988 MPI procs) for turbulence analysis: from turbulence fluxes and TKE budget to Boussinesq hypothesis validation,

Perspectives

- Development of boundary conditions able to mimic the presence of an exterior domain,
- Increasing the cavity’s height and/or increasing/decreasing the injection flow-rate in the objective to produce a two-layer stratification,
- Hydrogen-air cases.
Thanks for your attention!
3D flow description

Helium volume fraction

Velocity magnitude
Comparison of helium and hydrogen releases in 1 m 3 and 2 m 3 two vents enclosures: Concentration measurements at different flow rates and for two diameters of injection nozzle.

Experimental measurements, cfd simulations and model for a helium release in a two vents enclosure.
In *Proceeding of the International Conference on Hydrogen Safety*.

Large-eddy simulation of a turbulent buoyant helium plume.
*Bulletin of the American Physical Society, 53*.

CEA TRUST-TrioCFD (2017).
TRUST-TrioCFD code version 1.7.4.

Vertical turbulent buoyant jets: a review of experimental data.

Characteristics of small vortices in a turbulent axisymmetric jet.

The fluid mechanics of natural ventilation-displacement ventilation by buoyancy-driven flows assisted by wind.

Müller, B. and Muller, B. (1999). Low mach number asymptotics of the navier-stokes equations and numerical implications.


110 seconds of physical time,
> time evolution of the velocity magnitude at a point in the middle of top vent, quas—is steady solution assumed to be reached at 70 seconds.