PROGRESS IN URBAN AIR QUALITY ASSESSMENT:
CFD MODELLING OF A WHOLE TOWN IN SPAIN

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Introduction

Area of Study and Experimental Data

Modelling Approach
  - CFD model description and simulation setup
  - Numerical methodology

Results
  - Model evaluation with air quality monitoring stations
  - Model evaluation against experimental data from cyclists with microsensors

Conclusions
- **Urban air quality as big environmental problem**

- **Air pollution vs. human health**

- **Main source: The road traffic.**

Red and dark red dots correspond to values above the EU annual limit value and the WHO AQG (40 μg/m³). Only stations with > 75% of valid data have been included in the map (EEA, 2016a).

Perspective view of the wind lines in Pamplona when the wind blows North direction.

Result of the source apportionment analysis (annual NO2 mean for the whole Madrid municipality) (Borge et al. 2014).
LIFE-RESPIRA project goal: To improve urban air quality and reduce exposure to air pollution by promoting healthy and sustainable mobility.

Our LIFE+RESPIRA project task: To develop of an specific tool able to reproduce accurate pollutant maps of the Pamplona’s city (Spain).

Objective of this work: To compute the 2016 hourly $\text{NO}_2$, NO and NOx maps for annual and seasonal average days by means of a CFD-RANS methodology.
Area of Study and Experimental Data

Urban Morphology and Large-scale monitoring

Aerial view of Pamplona’s City
(Source: Google Earth)

Roads traveled by cyclists during 2016
(provided by University of Navarra)
CFD model description and simulation setup: Mesh Model

- **CFD Mesh model:**
  - Longitudinal plane section
  - CV_1
  - CV_2
  - **(*)**

- **Total number of cells:** $4.46 \times 10^6$

- **Zoom:**
  - $7 \cdot Z_{\text{max}}$ (***)
  - $1.5 \cdot Z_{\text{max}}$
  - $1.25 \cdot Z_{\text{max}}$
  - $5 \cdot Z_{\text{max}}$ (***)

- **Zmax:** 70m

(*) CFD tool: STAR-CCM+9.04.011®

(**) Franke et al. 2007
Modelling approach

CFD model description and simulation setup: Physical Models

- Steady State Simulations
- Segregated Flow Model
- RANS as turbulent approach:
  - Realizable K-ε Two-Layer model
  - All Y+ wall hybrid treatment
- Neutral atmospheric conditions
- Constant air density
- Default values of STAR-CCM + 9.04.011® as free parameters of the turbulent model
an additional passive scalar transport equation

Pollutant emissions at roads proportional to traffic intensity

Without atmospheric chemistry

\[
\left\{ \partial_j \left( \rho u_j C_{CFD}(\vec{r}) - \frac{\mu_{eff}}{S_{Ct}} \partial_j C_{CFD}(\vec{r}) \right) = S_C \right\}_{j=x,y,z}
\]

Daily Average Traffic Intensity map in Pamplona’s city
Modelling approach

CFD model description and simulation setup: Boundary Conditions

- **Building**: Solid boundary with surface specification: smooth
- **Ground**: Solid boundary with surface specification: roughness
- **Inlet**: $u(z) = \frac{u_* \ln \left( \frac{z + z_0}{z_0} \right)}{\kappa}$; $k = \frac{u_*^2}{\sqrt{C_\mu}}$; $\varepsilon = \frac{u_*^3}{\kappa \cdot (z + z_0)}$
- **Outlet**: $\Delta P_{in-out} = 0$
- **Top**: Symmetry boundary condition

(*) Richards & Hoxey 1993
Numerical Methodology (*)

CFD Simulations
\[ \{u_M\}_{i=1,\ldots,16} \] – scenarios

\[ \{C_{CFD,i}\}_{i=1,\ldots,16} \]

Meteorological Data: Pamplona GN Met. St. (**)  
\[ i\text{-scenario} \rightarrow \{f_i(t), \overline{u_{ref,i}(t)}\}_{t=1,\ldots,24} - \text{hour} \]

Pollutants Conc. Data: Pamplona Pza. Cruz A.Q. St. \( r_0^2 \)
\[ \left\{ \left( C_O(r_0^2, t) \right)_{NO_x}, \left( C_O(r_0^2, t) \right)_{NO_2}, \left( C_O(r_0^2, t) \right)_{NO} \right\}_{t=1,\ldots,24} \]

\( NO_x \) maps
\[
\left( C_M(t) \right)_{NO_x} = \left[ \sum_{i=1}^{16} f_i(t) \cdot C_{CFD,i} \cdot \frac{u_M}{u_{ref,i}(t)} \right] \cdot E(t)
\]
\[ E(t) : \left( C_M(r_0^2, t) \right)_{NO_x} = \left( C_O(r_0^2, t) \right)_{NO_x} \]

\( NO \) and \( NO_2 \) maps
\[
\left( C_M(t) \right)_{NO_2 \text{ or } NO} = \left( C_M(t) \right)_{NO_x} \cdot \frac{\left( C_O(r_0^2, t) \right)_{NO_2 \text{ or } NO}}{\left( C_O(r_0^2, t) \right)_{NO_x}}
\]

(*) Parra et al. 2010  
Santiago et al. 2013  
Santiago et al. 2017  
(**) Source: GN
High resolution hourly maps of NO$_x$ annual averaged concentration during 2016 at pedestrian level.
Model evaluation with air quality monitoring stations
Model evaluation with air quality monitoring stations: NO$_x$

<table>
<thead>
<tr>
<th></th>
<th>RE Max</th>
<th>Hour</th>
<th>R</th>
<th>NMSE</th>
<th>FB</th>
<th>FAC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2016-average annual day</td>
<td>55.5</td>
<td>2AM</td>
<td>0.843</td>
<td>0.080</td>
<td>-0.282</td>
<td>83.3</td>
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<tr>
<td>2016-average spring day</td>
<td>62.7</td>
<td>1AM</td>
<td>0.807</td>
<td>0.108</td>
<td>-0.298</td>
<td>70.8</td>
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<tr>
<td>2016-average summer day</td>
<td>50.1</td>
<td>11AM</td>
<td>0.666</td>
<td>0.108</td>
<td>-0.103</td>
<td>100.0</td>
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<tr>
<td>2016-average autumn day</td>
<td>55.9</td>
<td>4AM</td>
<td>0.826</td>
<td>0.099</td>
<td>-0.325</td>
<td>83.3</td>
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<tr>
<td>2016-average winter day</td>
<td>66.4</td>
<td>1AM</td>
<td>0.814</td>
<td>0.161</td>
<td>-0.439</td>
<td>70.8</td>
</tr>
</tbody>
</table>

NMSE < 1.5
− 0.3 < FB < 0.3

(*) Chang & Hanna 2005
Goricsán et al. 2011
## Model evaluation with air quality monitoring stations: NO\textsubscript{x}

### 2016-average annual day
- **Hour**: 5AM
- **R**: 0.890
- **NMAE**: 0.179
- **FB**: -0.094
- **FAC2**: 100.0

### 2016-average spring day
- **Hour**: 1AM
- **R**: 0.895
- **NMAE**: 0.214
- **FB**: -0.173
- **FAC2**: 100.0

### 2016-average summer day
- **Hour**: 3AM
- **R**: 0.811
- **NMAE**: 0.247
- **FB**: -0.187
- **FAC2**: 100.0

### 2016-average autumn day
- **Hour**: 5PM
- **R**: 0.860
- **NMAE**: 0.212
- **FB**: -0.097
- **FAC2**: 100.0

### 2016-average winter day
- **Hour**: 11PM
- **R**: 0.817
- **NMAE**: 0.245
- **FB**: -0.193
- **FAC2**: 87.5

**NMSE < 1.5**
- \(-0.3 < \text{FB} < 0.3\)

(*) Chang & Hanna 2005

Goricsán et al. 2011
Model evaluation with air quality monitoring stations: NO₂

<table>
<thead>
<tr>
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<th>RE Max</th>
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<th>R</th>
<th>NMAE</th>
<th>FB</th>
<th>FAC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2016-average annual day</td>
<td>59.1</td>
<td>1AM</td>
<td>0.683</td>
<td>0.250</td>
<td>-0.310</td>
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<tr>
<td>2016-average spring day</td>
<td>63.1</td>
<td>1AM</td>
<td>0.699</td>
<td>0.268</td>
<td>-0.321</td>
<td>70.8</td>
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<tr>
<td>2016-average summer day</td>
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<td>2AM</td>
<td>0.492</td>
<td>0.308</td>
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<td>2016-average autumn day</td>
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<td>5AM</td>
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<td>0.307</td>
<td>-0.396</td>
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<tr>
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<td>1AM</td>
<td>0.780</td>
<td>0.286</td>
<td>-0.364</td>
<td>75.0</td>
</tr>
</tbody>
</table>

NMSE < 1.5
− 0.3 < FB < 0.3

(*) Chang & Hanna 2005
Goricsán et al. 2011
Model evaluation with air quality monitoring stations: NO₂

<table>
<thead>
<tr>
<th>Pamplona-Iturrama</th>
<th>RE Max</th>
<th>Hour</th>
<th>R</th>
<th>NMAE</th>
<th>FB</th>
<th>FAC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2016-average annual day</td>
<td>53.7</td>
<td>1AM</td>
<td>0.754</td>
<td>0.296</td>
<td>-0.375</td>
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<tr>
<td>2016-average spring day</td>
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<td>1AM</td>
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<td>0.292</td>
<td>-0.370</td>
<td>83.3</td>
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<td>2016-average summer day</td>
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<td>0.741</td>
<td>0.392</td>
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<tr>
<td>2016-average autumn day</td>
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<td>4AM</td>
<td>0.853</td>
<td>0.346</td>
<td>-0.440</td>
<td>75.0</td>
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<tr>
<td>2016-average winter day</td>
<td>59.9</td>
<td>1AM</td>
<td>0.770</td>
<td>0.350</td>
<td>-0.427</td>
<td>75.0</td>
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</tbody>
</table>

NMSE < 1.5
-0.3 < FB < 0.3

(*) Chang & Hanna 2005
Goricsán et al. 2011
Model evaluation against experimental data from cyclists with microsensors

High resolution map of NO$_2$ annual average concentration during 2015 at pedestrian level

Annual average concentration map of NO$_2$ spatially-averaged in cells of 50 x 50 m$^2$

Comparison 50m-averaged CFD maps vs 50m-averaged cyclists maps presents several difficulties:

1. In CFD maps, the concentration represents the average value over all cell, while in cyclists maps, concentration represents the average value but only over the portion of the cell where the cyclists travel.

2. Measurements from cyclists are accompanied by a certain spatial uncertainty due to: the microsensors sampling time and the movement of cyclists. These instruments send data every 10 s (time-averaged concentration and GPS position), but during this period there are uncertainties about the actual GPS positions traveled by cyclists.

3. The total number of cyclists in some cells could not be enough to obtain a representative average concentration value.

Therefore, a direct comparison (point-by-point) seems not be suitable ...
Model evaluation against experimental data from cyclists with microsensors: NO₂, 8PM
Conclusions

- A CFD-RANS methodology has been modified and applied to the entire city of Pamplona to compute high resolution NOx, NO2 and NO maps at pedestrian level.

- This modelling approach is able to reproduce the data from air quality monitoring stations located within the domain, especially during daytime hours (from 8 A.M. up to 8 P.M.).

- Data from cyclists could not be directly compared (point-by-point), therefore a comparison by using a spatial statistical method that identifies clusters of high and low values of pollutant concentrations is applied. A preliminary analysis indicates that, in general, similar locations of maxima and minima of concentration are obtained in both, experimental and numerical maps.

- This methodology seems to be adequate to compute high resolution concentration maps for an entire city.
Thank you for your attention!

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