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CFD MODELING EVALUATION FOR REFINING ENVIRONMENTAL & SAFETY IMPACT CONCERNS

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Abstract: Computational Fluid Dynamics is a complex tool often used in design activity in fields of automobile, aeronautic or process by modelling flow behaviour. Using such a tool for atmospheric dispersion allows to take into account complex phenomena and very local site properties (buildings for example). Before optimizing computational time of such modellings it is important to develop physically coherent modelling with atmospheric physics able to tackle different atmospheric stability states. Indeed usual assumptions in CFD codes are not always compatible with atmospheric boundary layer description.

This work presents a validation of a specific set of parameters of the CFD code FLUENT for representing flow and gas dispersion within the Atmospheric Boundary Layer.

Impact of Refining activity comes from two main types of sources: canalized emissions (stack) and diffused or fugitive emissions.

CFD modelling will firstly be compared with typical Gaussian modelling and LIDAR measurements on a refinery plume in real operation and meteorological conditions. Such emissions are most of the time well modelled by Gaussian codes. Analysis focuses on plume rise and impact around site.

Diffused emissions are not very well described by standard tools especially for near-site impact assessment. CFD modelling results are, here, compared with Mock Urban Setting Test campaign on a specific case that is a situation closed to refinery diffuses emissions configuration with building influence.

Discussion will deal with CFD code weaknesses and ways taken to handle them. Moreover criticality of winds boundary condition in a building environment will be developed.

Key words: *CFD, dispersion modelling, MUST, Prairie Grass*

INTRODUCTION

Computational Fluid Dynamics is a complex tool often used in design activity in fields of automobile, aeronautic or process by modelling flow behaviour. Ability of CFD modelling to represent flow and gas dispersion for environmental Refining application is evaluated in present work.

METHODOLOGY

A specific methodology is used to model Atmospheric Boundary Layer (ABL) with Fluent code, it is described in details by Vendel *et al.* (2010). Key points are:

- Specific boundary condition at top of the domain (sky) to drive with the non-conservation of Reynolds tensor and Heat flux with use of symmetry BC
- Modified k-ε model with Duynkerke constants to make turbulence model coherent with Similitude theory.
- Use of pressure profile at exit boundaries and potential temperature profile at vertical boundaries.

PRAIRIE GRASS EXPERIMENT

The Prairie Grass experiment has been conducted in 1956 (...) and deals with real behaviour of gas emitted near ground on flat terrain. For this comparison try number 24 has been selected.

Meteorology

Stability condition of this case is <u>stable</u> and meteorology measurements give:

- Wind direction : 141 degrees
- Wind speed: 5.2 m/s
- Friction velocity: 0.41 m/s
- Sensible heat flux: -18.4 W/m²
- Temperature: 21.8 °C
- Monin Obukhov Length: 327 m

Emission

Source is a 46 cm height bottle emitting sulphur dioxide. Concentrations are 10mn averaged and measured at 1.5m above ground on arcs at distances of 50m, 100m, 200m, 400m and 800m. For the 24th case, SO_2 emission is 41.2 g/s.

Domain

Domain is rectangular with length of 1100m along the wind direction axis. Wind inlet is 200m before the source and width is 1000m. Height of domain is 150m.

Results

Results are represented on Figure 1 as comparison between measurements and modelling on 5 arcs at 50m, 100m, 200m, 400m and 800m from the bottle.

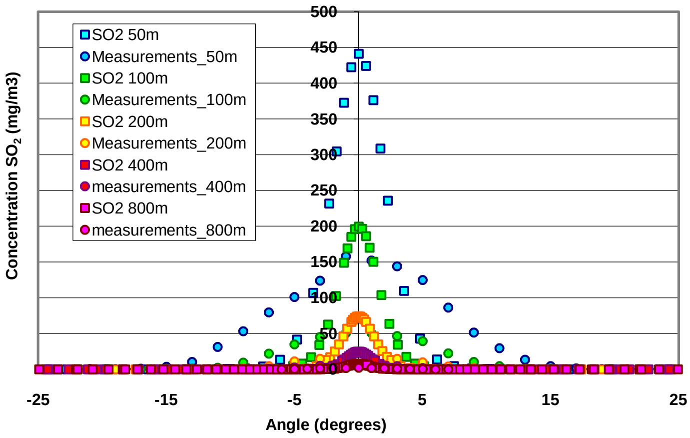

Figure 1: model / measure comparison on 5 measurements arcs

Modelling underestimates dispersion and leads to over estimation of SO_2 concentration on plume axis and under estimation of lateral spread.

Discussion

This difference comes from the fact that our modellings do not take into account direction variability on temporal scales larger than atmospheric turbulence scale. Our model is stationary and represents instantaneous concentrations. 10mn averaged measurements integrate direction variability that our modelling could not represent.

CFD modelling could not be compared to integrated measurements without a specific treatment of wind variability.

INDUSTRIAL LIDAR CAMPAIGN

A LIDAR (Light Detection And Ranging) measurements campaign has been conducted in TOTAL Refinery of Normandy in 2006. It aimed to observe pollutant plumes behaviour. For model/measures comparison we consider a specific SO_2 measure in a vertical plane that crosses plumes of certain stacks in south wind conditions.

Meteorology

Meteorology measurements come from Sandouville surface station and sensible heat flux comes from previous ADMS modelling on the same case:

- Wind direction : 222 degrees
- Wind speed: 7.1 m/s
- Sensible heat flux: -30 W/m²
- Temperature: 11.6 °C

Atmosphere is stable.

Emission

SO_2 emission and ejection parameters have been provided by refinery. 8 stacks are considered, characteristics are detailed in Table .

Table 1: source description

Source	Height (m)	Diameter (m)	Ejection velocity (m.s-1)	Ejection Temperature (°C)
Stack 1	29	1.9	7.8	370
Stack 2	65	2.56	9.4	272
Stack 3	75	0.9	8	310
Stack 4	65	2.6	8	489
Stack 5	110	4.46	9.5	289
Stack 6	65	1.7	4	460
Stack 7	80	1	1	450
Stack 8	80	5	10	300

Domain

A numeric mock up of a refinery is used to model this case. Geometry characterization is made thanks to buildings IGN (Institut Géographique National) data and the domain is meshed by 3.7M cells.

Results and Discussion

Modelling results are compared with LIDAR measurements on a vertical plane crossing the refinery's plumes. It will give us a critical advice of vertical and lateral dispersion. Furthermore LIDAR measurements are considered as instantaneous data. On Figure , LIDAR measurements are represented on a vertical plane with colour scale described in legend and modelling results are represented with an iso-surface of 200 µg/m^3 concentration.

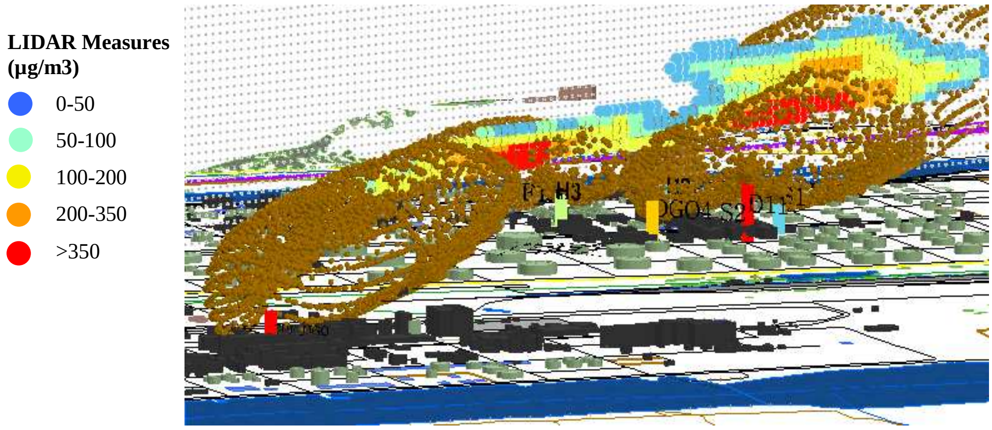

Figure 2: SO_2 modelled plumes compared with LIDAR measurements

This qualitative comparison shows a good agreement between modelling and measurements. The 2 zones of high concentration are well reproduced and are crossed by modelled plumes. Comparison between modelled concentrations of 200µg/m^3 and measured concentrations are coherent and confirms a good modelling of elevation and dispersion in first meters.

A more quantitative evaluation is made thanks to graph on Figure . Focus is done on east high concentration zone. Results are reported on a vertical plane and are represented with the value of concentration (colour) function of height above ground and distance to a point that corresponds to the position of LIDAR disposal.

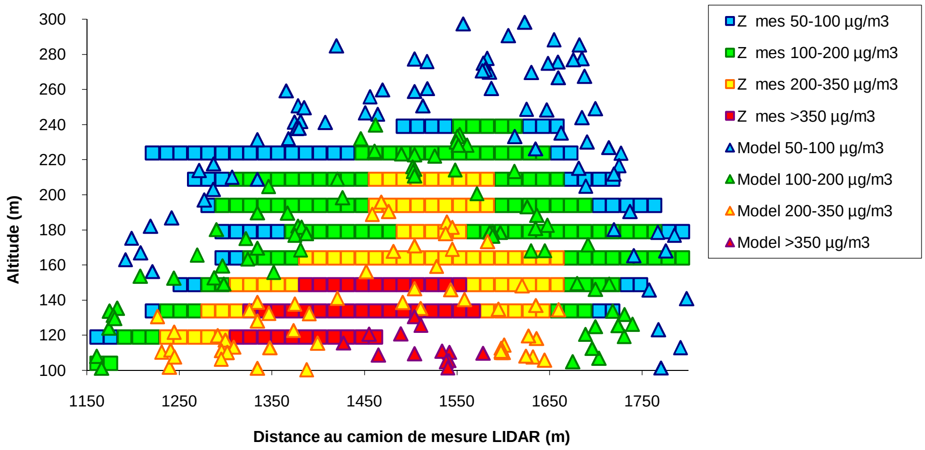

Figure 3 : model / measures comparison on measurement plane

Comparison shows a good agreement between modelling and measurements. Width and height of plumes are comparable and give good confidence in our model. This means too that elevation plume and close dispersion are well modelled.

MOCK URBAN SETTING TEST

MUST campaign was initiated by US Army in September 2001. It consists of dispersion measurement within a setup of buildings represented by 120 containers 2.54m high, 2.42m wide and 12.2m long. We selected the case of 19th Sept, 03:32 am.

Emission

Source is a horizontal tube at 0.15m above ground emitting propylene. It is located between 4 containers. Characteristics are the following:

- Type B
- Height above ground: 0.15m
- Emission duration: 16 min
- Flow rate: 200 l/min

Meteorology

Meteorology is measured on site close to the buildings grid, upstream of the source, on captor D at 6m above ground. For the selected case, data available allow us to determine mean direction, velocity and their standard deviation.

- θ_{moy} = 141.53 deg, σ_θ = 7.81 deg
- U_{moy}= 2.43 m/s, σ_U = 0.303 m/s

Atmospheric stability is evaluated thanks to average on 3 ground stations of LMO measurements at 2m above ground. The value is 19.7m, this is a stable atmosphere.

Fluctuations

Propylene concentrations and meteorology have been measured at high frequency and reveal significant variability during try. A correlation between wind direction variations and measured concentration fluctuations has been identified.

Those fluctuations will be modelled thanks to a transient approach using the code FLUENT. This approach uses the following hypothesis:

- there are two scales of fluctuations: under the minute (few seconds) and minute
- period of first scale variation is evaluated at 4.4s based on first minute measurements
- LMO is constant all along the try

For each minute direction and wind speed are written as

$$\theta = \theta_{moy} + 2\sigma_\theta \sin\left(\frac{\pi}{T}t\right) \text{ with } \theta \text{ the instantaneous angle} \tag{1}$$

$$\begin{cases} u = -\left(\dfrac{u_*}{\kappa}\left(\ln\left(\dfrac{z+z_0}{z}\right)+5\dfrac{z}{L_{mo}}\right)+2\sigma_U \sin\left(\dfrac{\pi}{T}t\right)\right)\cdot\cos\left(\dfrac{\pi}{180}\theta\right) \\ v = -\left(\dfrac{u_*}{\kappa}\left(\ln\left(\dfrac{z+z_0}{z}\right)+5\dfrac{z}{L_{mo}}\right)+2\sigma_U \sin\left(\dfrac{\pi}{T}t\right)\right)\cdot\sin\left(\dfrac{\pi}{180}\theta\right) \end{cases} \tag{2}$$

Except few extreme values there is a good agreement between modelled wind inlet and real measurement. In FLUENT transient simulation, time step is set at 0.22s.

Domain

Modelling domain is 400x400m wide and 20m high. A specific refinement is made close to the propylene source. A total of 2M cells are used.

Specific values of used physical parameter are summarized in Table .

Table 2: used parameter values

ρ	u*	z_0	C_p	θ_0	C_μ	z_t	μ	θ*	H_0
1.225 kg/m^3	0.123m/s	0.01m	1006 J/kg/K	283.9 K	0.033	0.0204m	1.7894E-05 Pa.s	0.05K	-8.212 W/m²

Results

A comparison between instantaneous measurements and instantaneous modelled concentrations has been made. Figure illustrates this comparison for the point dn26. Conclusions are:

- For each observation point, modelling gives the good variability of concentrations compared with the measurements.
- Impact levels are well modelled
- Main errors are observed on more de-centred points taking into account the relative position of the source and wind direction.
- The closer the source is, the higher the error
- Main reason of error seems to be the modelling of boundary condition (constant period)
- For far points but within the experimental site, comparison measurements / modelling gives very good agreement in terms of concentration levels and variability.

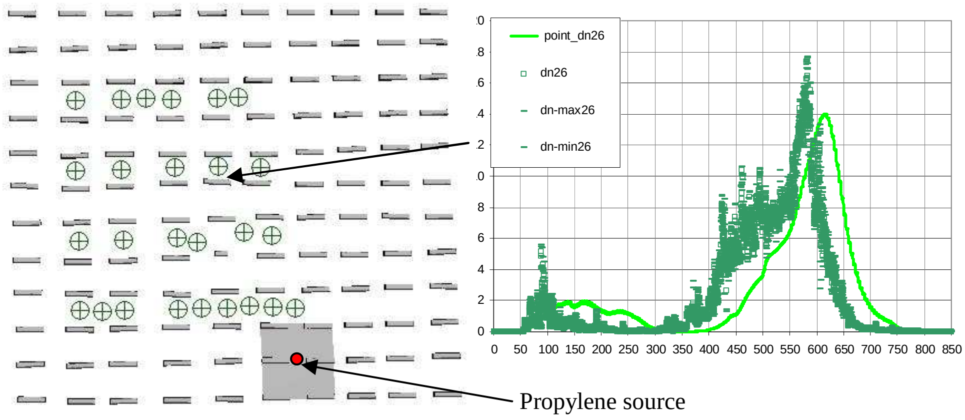

Figure 4: instantaneous concentrations at a specific observation point

Figure represents averaged concentration modelled and measured on the whole try period on each observation point with one colour per measurements line.

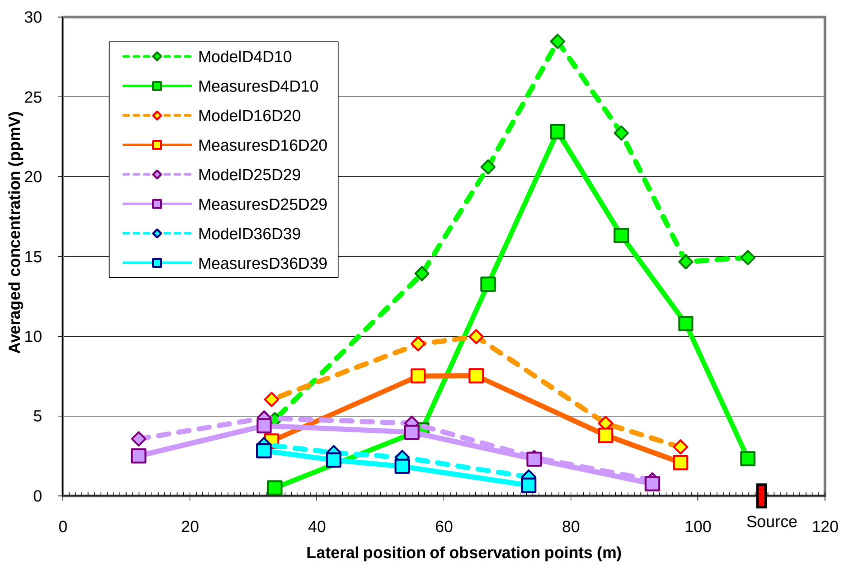

Figure 5: averaged concentration: model / measures comparison

Impact repartition is well modelled except for the D4 point which is very sensitive to real variability of wind direction. Modelled concentrations look to be slightly over estimated. Gaps are smaller when observation is far from the source.

CONCLUSIONS

CFD modelling has been evaluated for atmospheric dispersion modelling on real cases, adaptable to refining environmental and safety concerns. Results using a specific methodology have been compared with measurements.

Results of stationary approach over estimates integrated measurements but give good representation of instantaneous plumes. Transient simulations in a building environment have been conducted and comparison with MUST experiment gave rather good results. Concentration variability is well reproduced and averaged concentration is similar to averaged measurement.

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