

CFD SIMULATION OF THE THREE-DIMENSIONAL EFFECTS INDUCED BY THE NO_x PHOTOCATALYTIC DEGRADATION AROUND AN ISOLATED BUILDING

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ABSTRACT

In order to handle a case of pollutant dispersion in an urban environment Computational Fluid Dynamics (CFD) emerges as a fast and flexible method. By coupling it to a parametric optimization approach, the present study aims at simulating the photocatalytic destruction of NO_x particles as they hit the coated walls of an isolated building. This approach permits to evaluate the impact of different design parameters as the wind speed and the sun exposure on the air quality.

The first and critical step of the study presented in this article is to verify the CFD model. The focus is hence on determining, based on a comparison to a benchmark, the most appropriate physical model and spatial resolution to correctly represent fluctuating quantities, natural convection and particles diffusion. One important conclusion is that wall resolved modelization is required, as using wall functions leads to high overestimation of the pollutant destruction. After this first step, a design of experiments is carried-out to highlight the coating's ability to reduce pollutant levels according to its intrinsic properties, wind intensity and solar radiation. Effects of these parameters on the convective heat transfer coefficients are studied as well. Two metamodels are build, based respectively on 2D and 3D simulations. It appears that 3D effects cannot be neglected and that the freestream velocity is the most contributing factor in the air depollution rate, far ahead of the coating intrinsic depollution characteristic.

INTRODUCTION

Under UV irradiation, titanium dioxide (TiO_2) is a very efficient photocatalyst leading to the degradation of organic species (Henderson, 2011). As a result of catalytic heterogeneous reactions between titanium dioxide, water vapor and nitrogen oxides, NO and NO_2 molecules are transformed into HNO_3 . These highly reactive gases (NO_x) are formed when fuel is burned at high temperatures, released by vehicles for example. They cause a wide variety of health and environmental impact. Consequently, these depollution capabilities have led to a number of applications which benefit from the photocatalytic properties of TiO_2 , such as concrete pavements for example (Ballari et al., 2010).

In particular, these have been widely used in so-called de-polluting building materials, with the objective of removing the nitrogen oxides from the atmosphere.

For instance, an efficient decomposition was observed on the photocatalytic samples for TiO_2 doped commercial paints (Laufs et al., 2010). In addition, this study concluded that the painted samples do not represent a source of nitrous acid (HONO), which would have a negative environmental impact. The laboratory tests have shown that for very weak concentrations, the reduction in pollutant concentration can be approached by a linear equation which approximates the classical Langmuir-Hinshelwood decomposition. Decontamination efficiency, given by the factor k , becomes a measurable parameter characteristic of the coating.

This study is carried-out within the frame of a collaboration between Cenaero and AC&CS. AC&CS is currently working on the possibility of depolluting urban environment by applying a photocatalytic coating on exterior steel surfaces of buildings. Numerical simulations are performed by Cenaero to investigate the potential of such a product, with the aim of quantifying its effect on pollutant concentration.

This brings us to consider a problematic that is of major concern in building physics, related to convective heat exchanges at exterior building surfaces. Indeed, hygrothermal analysis of building components require the knowledge of the convective heat transfer coefficients (CHTC). These will also have a significant contribution in the photocatalytic reaction that occurs at the wall. Particular attention will be given to the flow resolution approach in the near-wall region, which was shown to play a critical role (Blocken et al., 2009).

The objective is to deeply investigate the physical phenomena that characterize the destruction process. The influence of various numerical parameters such as spatial discretisation will be analyzed. To best-perform these sensitivity analyses, the problem is simplified down to the case of an isolated building, subjected to a stream of uniformly polluted air that is partially depolluted by its coated surfaces. To justify the industrial interests in this product, the aim is to highlight the coating's ability to reduce pollutant levels by quantifying its impact on the building's close surroundings. A design of experiment is performed to understand the interactions between the different dependent variables. Due to time restrictions and considering the number of computations required, solving the steady RANS equations seems to be the only reasonable approach available to us. However, flow around buildings are

characterized by complex flow features with several separation areas.

It is therefore essential to first verify this approach against experimental data to ensure that the most relevant physics is correctly modelled. For this purpose, 3D numerical results are compared to wind tunnel data obtained for a given geometry. A series of sensitivity studies are then performed on the 2D geometry, focusing on mesh characteristics in particular. This is also an opportunity to deeply investigate the local flow and thermal characteristics for different convection regimes. Finally, a design of experiment is carried-out to approximate the problem. Based on the obtained meta-model, the photocatalytic process is analyzed in 2D and 3D in order to determine the importance of three-dimensional effects, based on a variance analysis which highlights the most contributing factors.

VERIFICATION OF THE CFD APPROACH

As mentioned previously, the steady RANS approach is the only possible method considering the limited computational resources available. The aim of this section is to verify that this approach is sufficient to represent the main flow characteristics in the region of interest, corresponding to the building's close surroundings, where the photocatalytic process will take place. It is important to note that this verification is performed in isothermal conditions.

CFD model

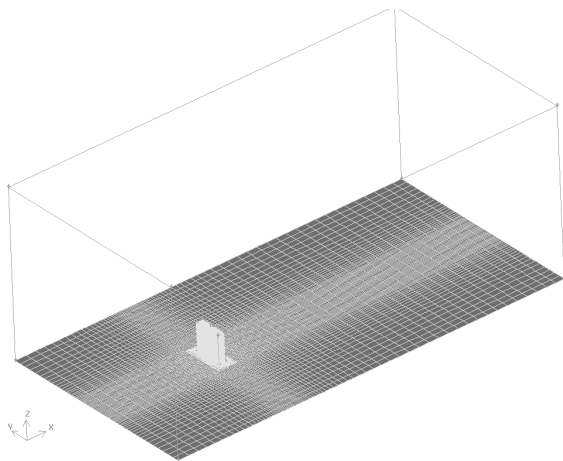


Figure 1: Computational domain ($-4H \leq x \leq 10H$, $-3H \leq y \leq 3H$, $0 \leq z \leq 6H$ with $H=20$ m) and ground mesh (y^+1 mesh)

The simulations are performed with the CFD package ANSYS Fluent 13.0 (ANSYS, 2009) Steady RANS equations are used and $k-\epsilon$ Realizable turbulence model is chosen due to its good performance for outdoor environment simulations (Blocken et al., 2011). The building, meshed in Gambit, measures 20 meters high and wide, and is 5 meters thick streamwise (see Figure 1). The wind is orientated along the x direction and remains fixed throughout the study. Recognized

guidelines (Franke et al., 2007) are used to define the size of the computational domain.

Two meshes were created in this verification phase, in order to study the influence of the near-wall approach on the results. The first mesh, denoted by y^+1 , is fine enough for the flow to be resolved down to the wall. This requires the first mesh point to be within the viscous sublayer, such that $y^+ \sim 1$ (first cell thickness of $y = 2.10^{-4}$ m), resulting in about 25 million cells. Alternatively, mesh y^+200 approximates the flow in the near-wall region by using a standard wall function. In this case, a y^+ value of about 200 ($y = 5.10^{-2}$ m) is used so that mesh size could be reduced down to approximately 0.8 million cells.

Experimental benchmark

The simulation is developed to match the wind tunnel testing conditions collected by the Architectural Institute of Japan (Tominaga et al., 2008). An atmospheric boundary layer is developed along the test section upstream of the scaled model, by using appropriate roughness elements and turbulence generators. To define inlet boundary conditions, the measured velocity and turbulent kinetic energy profiles are imposed. Steady RANS Velocity contours and streamlines in the symmetry plane (xz) are shown on Figure 2. As we can see, the presence of the building naturally creates a large recirculation bubble in its wake, of about three building heights, caused by flow separation at the front upper corner of the building. As the flow circulates upwards along the rear wall of the building, it separates at roof level, inducing a reversed flow region covering the roof. Small recirculations also appear at the foot of the building upstream and downstream.

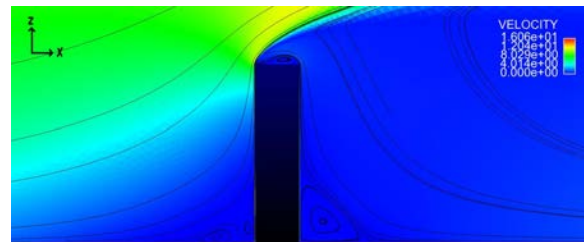


Figure 2: Steady RANS Velocity contours [m/s] and streamlines in the symmetry plane (xz)

A quantitative comparison of the flow is carried-out in between numerical and wind tunnel results. Both meshes y^+1 and y^+200 are confronted to determine the influence of the near-wall approach. The chosen quantities of interest are the horizontal velocity component and the turbulent kinetic energy. These are compared along vertical lines spread out along the symmetry plane at different distance from the building (building downwind face, $x = 2.5m$ and 5 cm from this face, $x = 2.55m$). First of all, it appears that the near-wall approach has a negligible influence on the flow characteristics. Velocity profiles are similar (Figure 3) and small discrepancies are observed for

the turbulence levels. We may conclude that resolving the flow down to the wall is unnecessary as it hardly affects the results against a substantial increase in computational time. However, it is important to note that this conclusion is valid only for isothermal flows, and remains to be verified in the presence of thermal effects. This 3D benchmark has provided satisfactory results since differences between numerical and experimental results remain acceptable. Indeed, within an industrial context, these are reasonable considering that the aim is to study the behavior of the photocatalytic coating. The computational requirements associated to more advanced CFD approaches such as LES or DES remain out of reach, and are not considered relevant for this application.

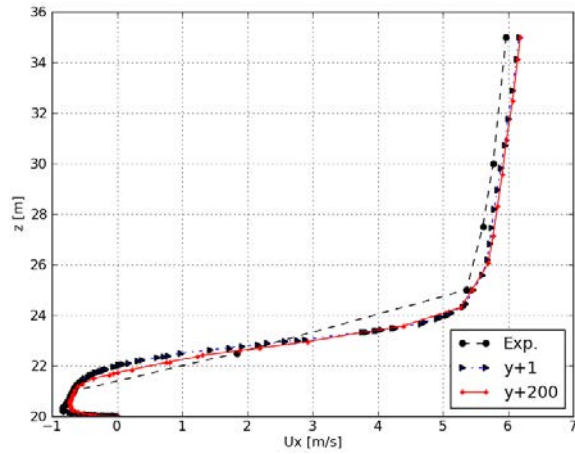


Figure 3: Comparison with the experiment of the velocity profile (U_x) on the top of the building roof, at the downwind corner ($x = 2.5$ m) [m/s]

SIMULATION

Due to time restrictions, the problem is simplified to two-dimensions in order to reduce the size of the domain. The simulations are hence representing the pollution dispersion and destruction around an infinitely long building. The thermal effects, neglected up to now, are added to the problem in order to simulate the presence of the coating and the photocatalytic reaction. The aim in this section is to determine what are the best-suited parameters to correctly represent the process.

Modeling of pollutant destruction

As this study does not aim at characterizing the chemical reactions between the air and the pollutant, these are neglected. In addition, the pollutant is considered to be simply transported by the flow without perturbing it, and is represented by a user-defined scalar (UDS). The pollutant is injected with a certain initial concentration C_0 at the inlet of the domain (at the inlet velocity boundary) and pollutant destruction is imposed by applying a flux boundary condition to the scalar along the exterior surfaces of the building. In addition, the effect of solar gain on the building is

taken into account via a heat source boundary condition at the wall.

Physical modeling

To select the best-suited physical model for the simulation, the importance of natural convection phenomena needs to be evaluated. We refer to the Richardson number, Ri , to estimate the importance of natural convection relative to forced convection induced by exposure to wind. This non-dimensional number is defined by the following equation: $Ri = gH/U_\infty^2$.

Considering that natural convection is negligible for $Ri \ll 1$ and dominant for $Ri \gg 1$, calculations are carried-out at three representative values of 0.1 (Ri_1), 1 (Ri_2) and 10 (Ri_3). The initial concentration C_0 is fixed to $4.06e^{-6} mol/m^3$ ($187\mu g/m^3$) and the surface heat flux to $400 W/m^2$. The corresponding free-stream velocities U_∞ , imposed at 135 meters high, are 25.6, 8.1 and 2.5 m/s respectively. We rely on velocity and concentration levels close to the building, as well as CHTC distributions along the building. Results using an incompressible model and a Boussinesq approximation, referred to by the index *noB* and *B* respectively, are compared on Figure 4.

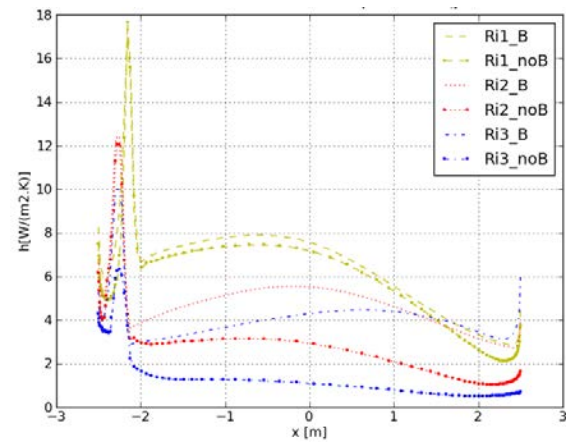


Figure 4: Boussinesq approximation effect on CHTC (h) of the roof for 3 Ri

As expected, it appears that taking into account natural convection effects becomes increasingly important as the Richardson number gets larger. For a Richardson number of 10 for instance, Figure 4 shows that the CHTC is under-estimated by an order of two while pollutant destruction is over-estimated by up to 30%. To conclude, it is fundamental to take these into account with appropriate physical modeling. In the coming parametric study, higher surface heat flux values might induce temperature differences too large for the Boussinesq hypothesis to remain valid. Therefore, it is recommended to select the 'incompressible ideal gas law' model.

Mesh dependency study

The influence of the near-wall approach is investigated, for a non-isothermal flow with pollutant destruction occurring at the wall. Non-dimensional con-

centrations are compared for meshes y^+1 (resolved) and y^+200 (wall function). We observe that a resolved mesh is essential to correctly capture the steep concentration gradient that originates at the wall, where the photocatalytic reaction takes place. As we can see on Figure 5, this mis-modeling impacts directly on the global pollutant levels in the building's close surroundings. A strong over-estimation of the de-pollution is predicted with mesh y^+200 , such that the use of a resolved mesh is inevitable. However, to ensure that all flow characteristics are fully resolved, it is important to verify what would be the boundary layer thicknesses related to not only the dynamic effects, but also thermal effects and pollutant diffusivity. Each of these are characterized by non-dimensional numbers, namely the Reynolds (Re), Prandtl (Pr) and Schmidt (Sc) number. Considering that $Pr \sim 0.7$, thermal and dynamic boundary layers are similar. To evaluate diffusive effects however, the diffusivity coefficient and turbulent viscosity should be of the same order of magnitude. These have been compared and are indeed of the same order, which confirms that a y^+ value of ~ 1 (at most a y^+ value of 4 was obtained) is sufficient to resolve all different flow phenomena.

This $y^+ \sim 1$ mesh with incompressible ideal gas law model will hence be used in the next step, in the Design Of Experiments.

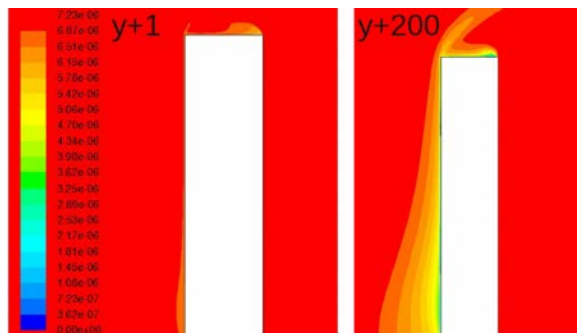


Figure 5: Comparison of the pollutant concentration levels (UDS contours) for different mesh refinements: with a near-wall approach ($y^+ \sim 1$ on the left) or with a wall function ($y^+ \sim 200$ on the right)

DESIGN OF EXPERIMENTS

Methodology

We recall that this study aims at determining the influence of a number of flow and coating parameters on the coating's ability to reduce the pollution levels around an isolated building. The 2D sensitivity analyses presented previously have clearly established the need to use a resolved mesh. However, this induces a very large mesh which would require an important computational effort to reach a converged solution. Consequently, performing a parametric study in a classical way, by looking at the independent effect of each input parameter, would require too many computations. An alternative to this approach is to construct a so-called 'Metamodel' that approximates the CFD

model. It is based on a number of analyzed configurations, and although less accurate, it has the advantage of having a very low computational cost (analytical expression).

The optimization platform 'Minamo', developed at Cenaero, is used to approach the photocatalytic process, and replace the high-fidelity model. Let us describe the different stages necessary to reach a converged metamodel.

First of all, a space filling technique is used to distribute the samples homogeneously in the design space, given by variation intervals defined for each input parameter. Each sample is given by a set of input parameter values used to set-up the computation. Later on, the metamodel is enriched by using an adaptive training. More specifically, the Monte Carlo method that is used is a Latinized Centroidal Voronoi Tessellation (LCVT). It presents the benefit of adding samples in regions with higher non-linearities, which results in an optimized exploration of the design space.

The metamodel corresponds to a mathematical expression based on interpolation constructed on this limited number of samples. The quality of this surrogate model has to be regularly estimated in order to perform a proper training. For this purpose, a Leave One Out Cross Validation (LOOCV) is performed. As the name suggests, LOOCV involves the use of a single observation from the original set of samples as the validation data, and the remaining observations as the training data for the surrogate model. This is repeated so that each observation is used once as the validation data. Correlation coefficients are calculated between the predicted value given by the metamodel, and the actual CFD value. The model's quality is then estimated based on these values comprised between 0 and 1, 1 being a perfect fit.

Once the metamodel is considered as sufficiently representative, it can be exploited to extract information. For instance, the coating's behavior will be analyzed by performing an 'ANalysis Of VAriance' (ANOVA). This phase consists of a sensitivity analysis technique that performs a breakdown of the variance of a function into components dependent on each observed function. The results indicate the relative first and second order contribution of the different input parameter variations on the changes experienced by each output. Based on this information, we may conclude on which factors contribute the most to the photocatalytic process.

Finally, a more detailed analysis is possible by exploiting the metamodel to extract quantitative results. These can be obtained at a very low computational cost through 1D or 2D evaluations where only one or two of the inputs vary at a time.

Parametrization of the problem

Considering that solar gain cannot be perceived by all building walls simultaneously, the configuration is defined in order to be as realistic as possible. In addition

to the roof, only one of the vertical walls should be exposed at a time. We focus here on a case where the photocatalytic coating is applied to the rear facade and the roof. These two surfaces are referred to as 'active' and are subjected to solar heating (surface heat flux). In terms of relevant inputs to the problem, three parameters were identified as potentially having a relevant contribution to the process. These are given below along with their variation interval:

- wind intensity at roof height H V_{magn} , within [1.4 ; 11.4] m/s
- coating factor k , within [-100 ; -1] dm/min
- corrected solar heat flux Q_{corr} , within [100 ; 800] W/m^2

Several outputs are chosen to represent pollutant destruction. Several volumes are defined around the building, in which average concentrations are calculated. Three volumes are placed at pedestrian level (z : 0 to 5 meters high), and cover the building laterally (y : ± 10 meters wide). They all go from the building's rear facade ($x = 2.5$ m) and extend progressively further downstream, with:

- $p1$: x from 2.5 to 3 m \rightarrow 0.5 m long
- $p2$: x from 2.5 to 3.5 m \rightarrow 1 m long
- $p3$: x from 2.5 to 7.5 m \rightarrow 5 m long

A fourth volume $p4$ is positioned above the roof. It has the same dimensions than the roof and is 5 meters high. These four outputs are referred to as C_{p1} , C_{p2} , C_{p3} and C_{p4} respectively. Three additional outputs are defined as the average CHTC values along each building wall, noted h_{front} , h_{top} and h_{back} . Consequently, there are in total three inputs and seven outputs.

Strategy

The large computational cost associated to the 3D resolved mesh, of about a week on 7 processors, is considered as excessive for this study. To reduce its size, only half of the building is represented laterally, with a symmetry boundary condition applied to the cutting plane (x,z).

The two-dimensional model is also run in order to highlight the differences existing between the 2D and 3D models. This simplification is similar to assuming that the building is infinitely long ($L \gg$) in both lateral directions. However, since the length to height ratio (L/H) of the real building is equal to 1, this hypothesis is far from being valid in 3D. Therefore, we expect large differences in flow characteristics which will impact on the performance of the coating and the way it behaves with respect to the different input parameters.

DISCUSSION AND RESULT ANALYSIS

Three-dimensional flow effects

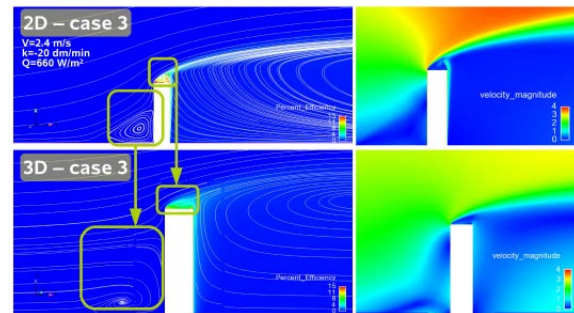


Figure 6: Comparison of 2D and 3D de-pollution rate contours (left - 0 to 15%) and velocity contours (right - 0 to 4 m/s) in the symmetry plane

The simplification from 3D to 2D implies that the flow cannot go around the sides of the building. A total blockage is produced such that the flow can only go past the building from above. At the contrary, the flow blockage is limited in 3D which will induce large differences between the 2D and 3D flow characteristics. These models are compared on Figure 6. The velocity contours on the right highlight important differences in velocity levels. Indeed, 2D flow blockage considerably slows down the flow in front and behind the building compared to the 3D case. As a result, a larger upstream recirculation bubble appears. In 2D, there is a general upward movement of the flow along the front facade (less pronounced in 3D since the flow goes partly sideways). This results in a larger recirculation region above the roof, which in turn induces stronger depollution due to a longer contact time between the air and the coating. Similarly, velocities are weaker at the back of the building. More generally, the velocities are lower in the building's close surroundings in 2D, which should induce weaker natural convection forces.

Leave-One-out

To obtain a high quality metamodel in 2D, where all correlation coefficients are above 85 %, 45 cases had to be resolved. In 3D however, due to computational limitations, a total of only 23 cases were run to construct the metamodel. The DOE is slower to converge because in 3D the average concentrations are calculated in volumes that cover the whole width of the building. However, the flow differs a lot between the building's extremities and the center, which induces different concentration levels. Consequently, lower correlation coefficients were reached. Despite lower correlation coefficients in 3D, all values are above 0.8 except for output C_{p3} (0.7). These remain acceptable since we are interested in having a first idea of the coating's efficiency range and the way it behaves with respect to the various input parameters.

Analysis of variance

Behavior of CHTC values

A linear law (ISO13790, 2008) is frequently used in building physics to calculate the CHTC value. It is directly related to the free stream velocity at 10 meters high, by:

$$h_c = 4 + 4V_{magn,10m} \quad (1)$$

One of the objectives in this study is to approximate the behavior of the three CHTC outputs and compare the results to this law. To achieve this, an analysis of variance is performed as presented in section . Both series of results are compared on Figure 7. These indicate how much each input parameter (V_{magn} , k and Q_{corr}) influences each CHTC value.

In 2D, we observe that the CHTC values obtained on the roof and especially the back facade of the building strongly depend on the solar heat flux Q_{corr} . Only the front coefficient h_{front} evolves linearly as a function of free stream velocity V_{magn} , whereas in 3D all CHTC values do. These observations can be explained by the fact that in 3D, flow characteristics are partly governed by V_{magn} due to limited blockage. Lateral and wake recirculations are therefore influenced by the free stream, which in turn dominate heat transfer exchanges at the wall. The opposite occurs in 2D, where total blockage of the flow sideways considerably reduces the influence of V_{magn} on these flow features. As a consequence, natural convection effects play an important role in these exchanges, particularly in the wake. Free stream velocity still dominates (71 %) over solar heat flux (27 %) above the roof since it affects the number and size of the recirculations.

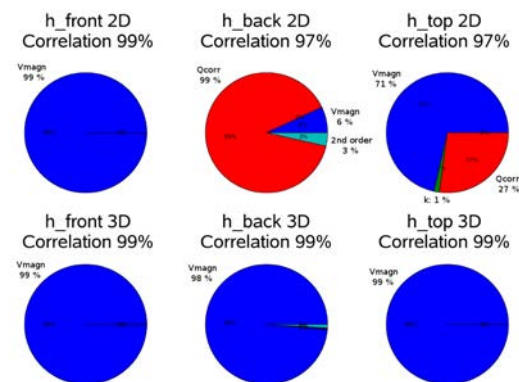


Figure 7: Comparison of the 2D (top) versus 3D (bottom) convective heat transfer coefficients ANOVA

To evaluate how the CHTC trends compare to the linear expression given by the standards, the two meta-models are exploited to represent how the facades and roof CHTC evolve as a function of V_{magn} only. The observations made previously based on an analysis of variance are confirmed by these 1D evaluations. The CHTC values in 3D depend solely on free-stream velocity and evolve linearly. In 2D, only h_{front} , directly exposed to the incoming wind, depends directly on V_{magn} .

As a result, the front CHTC values are given by the following expressions:

$$2D : h_{front} = 1.5 + 1.8V_{magn,10m} \quad (2)$$

$$3D : h_{front} = 2.3 + 2.7V_{magn,10m} \quad (3)$$

In 3D, the CHTC values are comparable to the standard values. It is once again due to total flow blockage that the slope observed in 2D departs further from the reference value of 4. Indeed, standards provide a relatively good indication in the case of a 3D isolated building. However, these results suggest that in more specific urban configurations such as street canyons, where important flow separation is expected, CHTC values will evolve differently as it is already the case in 2D.

Pollutant destruction

In terms of concentration levels at pedestrian level, similar observations can be formulated. The graphs provided by the analysis of variance are shown on Figure 8. These show that in 2D, pollutant destruction in the wake of the building is strongly influenced by natural convection effects (solar heat flux dependency). The contribution of output C_{p1} reaches 59 %, while the coating's factor k and V_{magn} are limited to 18 % and 19 % respectively.

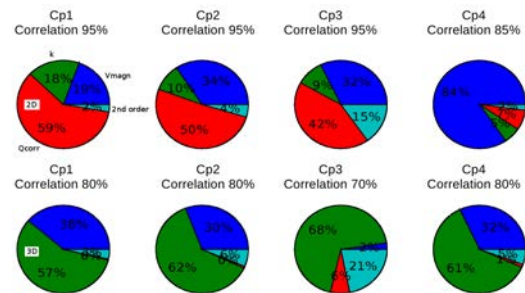


Figure 8: Comparison of the 2D (top) versus 3D (bottom) pollutant concentrations ANOVA (concentrations averaged in volumes 1 to 4)

As the volume extends further downstream, from volume p1 to p3, flow properties (V_{magn}) grow in importance while the opposite is observed for surface properties (k and Q_{corr}). The contribution of free stream velocity increases up to 32 %, whereas the values of k and Q_{corr} drop down to 9 % and 42 % each.

The same behavior is observed in 3D, however quantitative trends are very different. In agreement with previous remarks, natural convection effects are limited due to free stream dependency in the wake. Therefore, as opposed to 2D solar heat flux has a negligible influence. Instead, coating property k dominates over free stream velocity, with contributions of 57 % and 38 % respectively in volume p1.

Finally, in the region above the roof covered by volume p4, depollution is mainly sensitive to V_{magn} in

2D (84 %). In 3D, the coating itself contributes much more (61 %) than freestream (32 %).

Just like for CHTC values, a quantitative analysis is performed by exploiting the two metamodels. In both cases, depollution decreases as we get away from the building since the photocatalytic reaction takes place locally at the wall. Nevertheless, while in 2D the reaction's efficiency improves as freestream velocity increases, the opposite occurs in 3D, as we can see on Figures 9 and 10.

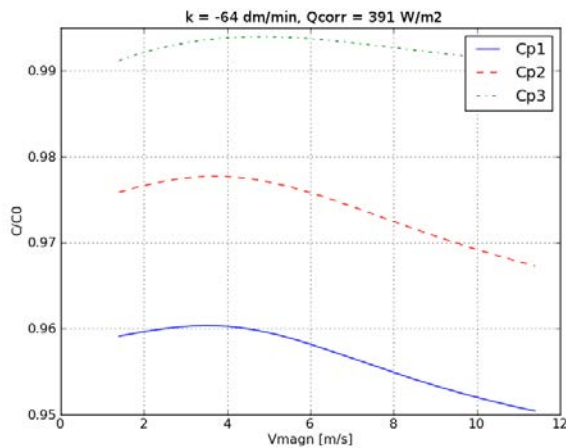


Figure 9: Effect of the freestream velocity (V_{magn}) on the nondimensionalized pollutant concentrations (C/C_0) in 2D

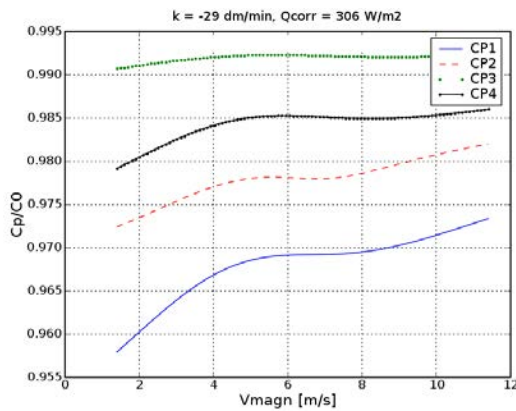


Figure 10: Effect of the freestream velocity (V_{magn}) on the nondimensionalized pollutant concentrations (C/C_0) in 3D

In 2D, the blockage effect helps to explain this behavior since the higher the incoming wind speed, the stronger the blockage. As a consequence, velocities in the wake are reduced which implies a longer contact time between pollutant and rear surface. Thus pollutant destruction gets stronger as freestream velocity increases. In both cases, a maximum destruction of approximately 6 % is reached in volume p1.

Figure 11 shows how in 2D coating efficiency deteriorates with increased solar heat flux. Indeed, natural convection forces the flow to move upwards along the rear wall. The flow accelerates with solar gain, and the contact time decreases which leads to less destruction.

In 3D, it is the coating factor k that dominates, where logically (ref. Figure 12) destruction increases with k (in negative). However, we notice the presence of a saturation window, corresponding to a value beyond which destruction efficiency deteriorates. For instance in this case, the destruction remains stable beyond a value of about -50 dm/min, meaning that having a larger absolute k value is unnecessary as it does not induce any further destruction. This same figure also indicates that depollution above the roof is stronger than at pedestrian level in the wake (C_{p4} compared to C_{p3} , simply because the air comes from the wake region and has already been partially de-polluted.

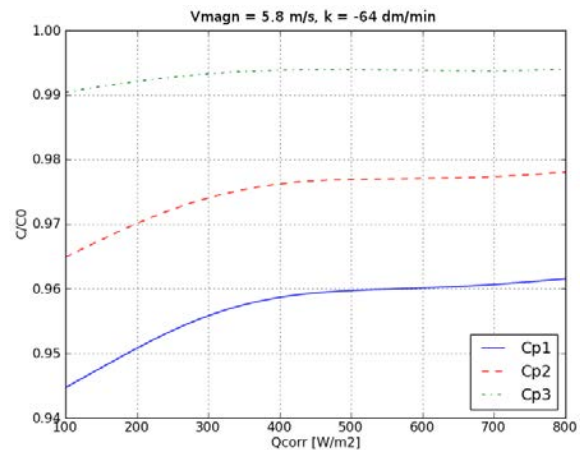


Figure 11: Effect of the solar gain (Q_{corr}) on the nondimensionalized pollutant concentrations (C/C_0) in 2D

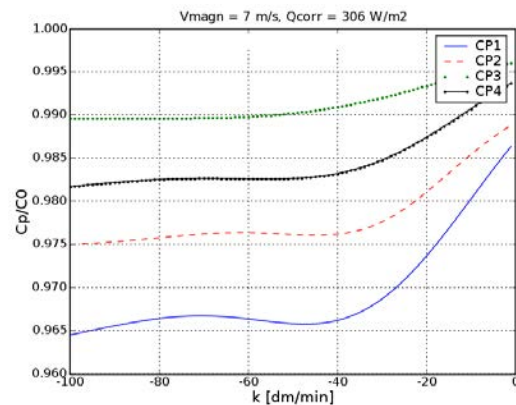


Figure 12: Effect of the photocatalytic coating property (k) on the nondimensionalized pollutant concentrations (C/C_0) in 3D

CONCLUSION

The study of pollutant dispersion and destruction by photocatalytic reaction occurring on the exterior surfaces of an isolated building was investigated numerically. A steady RANS simulation was performed with the software ANSYS Fluent.

The CFD method was verified in 3D by confrontation to wind tunnel data. Results indicate that in isothermal conditions without pollutant dispersion, a RANS

approach with a standard wall function is sufficiently precise to characterize the flow in an industrial framework. Particular attention was brought to the building's close surrounding, of particular interest in this project.

A detailed analysis showed however that to correctly model pollutant destruction at the wall, the flow had to be resolved in the near-wall region instead of being approximated by a wall function. An alternative would be to develop a customized wall function that would be appropriate to represent the user-defined scalar in this region. In the perspective of simulating the flow within an entire neighborhood, this would be an essential measure to maintain a reasonable computational effort.

A 2D analysis highlighted the importance of thermal effects, and of natural convection forces in particular. These act on flow characteristics which in turn will impact the coating's efficiency. This is particularly true as natural convection takes over forced convection at lower speeds. Consequently, an incompressible ideal gas solver is best suited to model problems defined by larger temperature gradients.

A parametric study was carried-out in order to highlight the role played by the coating factor, the surface heat flux due to sun exposure and incoming wind velocity. The focus was on their impact on depollution and convective heat transfer coefficients at the wall. Thanks to the Minamo software, a design of experiments was performed so that the number of evaluations could be greatly reduced. This approach brought considerable added value to the study. The design space was efficiently scanned and post-processing of the results allowed us to identify the most contributing factors thanks to an analysis of variance. Eventually, the high-fidelity model could be replaced by the metamodel to cheaply extract further information. Various evaluations, where only one input parameter would vary at a time, help distinguish tendencies and obtain quantitative results.

The comparison of 2D and 3D metamodels showed that three-dimensional effects are significant. Flow blockage in 2D has a considerable impact on coating behavior. In 3D, freestream velocity remains the most contributing factor, while results depend strongly on solar heat flux in 2D (natural convection effects).

In terms of CHTC values, results highlight their sensitivity with respect to the configuration. Standards may provide a good indication for an exposed surface but most often these depend on local flow characteristics. For instance, 2D values even along the windward surface are strongly reduced due to flow blockage.

As for the destruction process is concerned, depollution reaches at most 6 % in average, within a volume that extends from the rear wall to half a meter downstream (5 meters high). Once again, flow features play a critical role on the coating's behavior. The 2D/3D comparison illustrates this dependency; as it was the

case for CHTC values, freestream velocity strongly dominates in 3D whereas natural convection is significant in 2D.

This study has given a first indication of the coating's behavior and efficiency. Based on these results obtained for an isolated building, the objective would be to benefit from these outcomes and extend simulations to first a street canyon and eventually a small neighborhood. One of the challenges would be to develop an appropriate wall function to approximate the pollutant's behavior in the near-wall region. This would reduce the size of the computational mesh down to a reasonable size. An alternative could be to only resolve the near-wall regions that are coating.

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