CFD SIMULATION OF AEROSOL DEPOSITION IN APSLEY HOUSE, LONDON

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ABSTRACT

We implemented an Eulerian model of aerosol dispersion and deposition in a commercial CFD code (Ansys Fluent). We used this model to simulate the penetration, dispersion and deposition of particulate matter of outdoor origin (larger than 1 μm) in a naturally ventilated historical building (Apsley House, London). The ingress of particles through cracks in the building envelope is estimated using a penetration factor model implemented into the CFD code. We investigate the effects of wind induced leakage, forced and natural ventilation. Our approach successfully predicts the spatial variation of deposition, and offers reasonable estimations of maximum and minimum yearly average deposition rates. Considering only ventilation, the deposition velocity v_d = $2.6\times10^{-4}\pm8.6\times10^{-5}$ s^{-1}, considering only leakage, v_d = $6.6\times10^{-5}\pm4.18\times10^{-5}$ s^{-1}. Both values are within the experimentally determined range, with a maximum of v_d = 1×10^{-4}, minimum of v_d = 9.2×10^{-6}, and average of v_d = 2.1×10^{-5} s^{-1}.

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INTRODUCTION

During the last two decades several models of aerosol dispersion and deposition on the scale of a building have been developed [K. Lai and Nazaroff, 2000, Nazaroff and Cass, 1989]. Health concerns are generally the motivation behind the development of such models and their application to real cases studies are generally focused on good predictions of the concentration of particulates in the free volume. Many of these models have also been successfully tested in experiments in controlled laboratory environments [Lai and Nazaroff, 2005, Hussein et al., 2009]. So far, such experimental validations have been carried out by measuring the decay rate of suspended particle concentrations. However, in some contexts, such as cultural heritage institutions (museums, archives or historic houses), concerns about particulate matter (PM) are not only related to the concentration in the bulk air, but specifically to the amount of particles that reach heritage surfaces, i.e. the deposition rates [Nazaroff, 1993].

In this work we present a prediction of deposition rates in a historical building, Apsley House, London, managed by English Heritage. This historical house is located at a very busy roundabout (Hyde Park Corner), and we can safely assume that pollutants in the size-range of interest are largely of outdoor origin. It is mostly naturally ventilated, however, air flow is controlled by forced ventilation in some rooms. The house has a complex environment that is affected by multiple factors. Some are a source of daily variation (such as road traffic or wind) while others cause long-term patterns (such as visitors or use of the ventilation system).

Despite this complexity, we describe a model to estimate deposition rates which only requires annual averages as initial inputs. We use representative values of pollutant fluxes through cracks, outdoor wind speeds and velocities in the ventilation inlets. We use steady-state simulations. Certainly, this approach requires a number of assumptions and simplifications which we explain and justify in detail throughout the text. Our aim is to assess whether Computational Fluid Dynamics (CFD) simulations can be used to obtain realistic and useful predictions of aerosol behaviour in complex environments. Our results will also determine whether and which additional pieces of information could improve the accuracy of predictions.

MATHEMATICAL MODEL

We divided the simulation in two stages. In the first stage, we investigated the fraction of outdoor aerosol that penetrates indoors through cracks and gaps in the building envelope. In this stage we used CFD simulations of the outdoor environment surrounding the house to obtain the pressure on the walls. In the second stage, we produced a CFD simulation of the indoor environment, where the penetration factors obtained in the first phase were introduced as boundary conditions. We simulated every stage separately and with different computational meshes. In both stages we solved the linear momentum balance equation to obtain the air velocity.

Penetration factor

We solved the model proposed by [Tian et al., 2009] to predict the penetration factors of spherical particles through rough building leaks. This model understands the penetration factor, P, as the proportion of particles of a given size that manage to penetrate through a gap without depositing on its internal walls. The model assumes that particles deposit on the walls due to gravitational settling and Brownian diffusivity. P is defined as the product of the penetration factors due to these separate phenomena:

$$P \equiv P_d \times P_g \tag{1}$$

where P_d is the penetration factor due to Brownian diffusivity and P_g due to gravitational settling. P_d is calculated with the following equation:

$$P_d = exp\left(-\frac{1.967\mathscr{D}L}{[H-2(0.45k+d_p/2)]^2u}\right) \tag{2}$$

where k is the wall roughness (a representative height of the surface irregularities), d_p is the diameter of the particles, L is the length of the crack (its depth towards the interior of the wall) and H is its height. $\mathscr{D}$ is the Brownian diffusivity which we approximated with the expressions detailed at [Grau-Bove et al., 2014] and u is the mean airflow, calculated as:

$$u = \sqrt{\Delta p + \left(\frac{1.208\times10^{-4}}{H^2L}\right)^2} - \frac{1.208\times10^{-4}}{H^2L} \tag{3}$$

where Δp is the pressure difference between the two sides of the crack, which is obtained from the CFD simulation of the outdoor environment.

We calculate the penetration factor due to gravitational settling with the following equation:

$$P_g = 1 - Lv_s/(H-d_p)u \tag{4}$$

where v_s is the settling velocity:

$$v_s = C\frac{\rho_p - \rho_f}{18\mu}gd_p^2 \tag{5}$$

The difference of pressure between the two sides of the wall is obtained from the CFD simulation. Atmospheric pressure has the same value indoors and outdoors. We also assume that the pressure on the indoor walls caused by internal ventilation is negligible in comparison with the pressure caused by wind on the outdoor walls. Under these assumptions, we can consider that the pressure difference through cracks in the walls is equivalent to the total pressure exerted by the wind:

$$P = \frac{1}{2}\rho_f u^2 + P_{static} \tag{6}$$

where P is the total pressure on the surface and P_{static} is the static pressure of the fluid.

Aerosol transport and deposition

In Ansys Fluent we implemented the drift-flux model for particle dispersion and deposition developed by [K. Lai and Nazaroff, 2000]. This model implies a series of assumptions on the flux: firstly, we assume that particles are vanishingly small, and therefore the Stokes number is close to zero and the aerosol can be treated as a scalar advected at the same velocity as the fluid phase (one way-coupling). Secondly, we assume that particles have a turbulent diffusivity which is very similar to the fluid turbulent viscosity. We also assume that particle coagulation is negligible. These assumptions are only valid within certain ranges of particle diameters, air velocities and turbulence, which we will assess in more detail in the following sections. As long as these assumptions hold, we can describe aerosol movement with the following equation:

$$\partial_t c = -\partial_x \cdot c(\boldsymbol{u} + \boldsymbol{v}) + \partial_x \cdot (\mathscr{D} + \varepsilon)\partial_x c \tag{7}$$

where c is the aerosol number concentration, $\mathscr{D}$ is the Brownian diffusivity and ε is the turbulent diffusivity of the aerosol, $\boldsymbol{u}$ is the velocity of the particle phase, and $\boldsymbol{v}$ is the settling velocity of the particles. A relevant feature of the model is that deposition is implemented as a boundary condition for the aerosol phase. Deposition is described as the total flux towards the surfaces and is defined with as:

$$J = -(\varepsilon + \mathscr{D})\frac{\partial c}{\partial n} + (\boldsymbol{v} \cdot \boldsymbol{n})c \tag{8}$$

where J is the flux of particles entering the wall, $\partial c/\partial n$ is the partial derivative of the aerosol concentration in the direction normal to the wall, $\boldsymbol{n}$ is the unit vector normal to the wall and pointing outside the domain, and therefore $(\boldsymbol{v} \cdot \boldsymbol{n})$ is the component of the settling velocity normal to the wall. We calculated the flux J with the constitutive equation developed by [K. Lai and Nazaroff, 2000] written in terms of bulk variables.

We have already discussed all the balance and constitutive equations elsewhere [Grau-Bove et al., 2014], together with the boundary conditions and an implementation strategy. Here we follow the same approach.

Turbulence is simulated using the RNG $k - \epsilon$ model available in Fluent by default. The choice of this model is based on preliminary laboratory experiments in a simpler geometry [Grau-Bove et al., 2014].

Applicability of the fluid dynamics model

The applicability of the model can be related to a set of dimensionless numbers, as we demonstrated in our previous work [Grau-Bove et al., 2014]. Here we investigate the value of this parameters in the current system. Perhaps the most relevant parameter defining the applicability of the drift-flux model is K_{pt}, which describes the ability of the particles to be transported by all the scales of turbulent motion.

$$K_{pt} = \frac{\tau u_{rms}}{l} \tag{9}$$

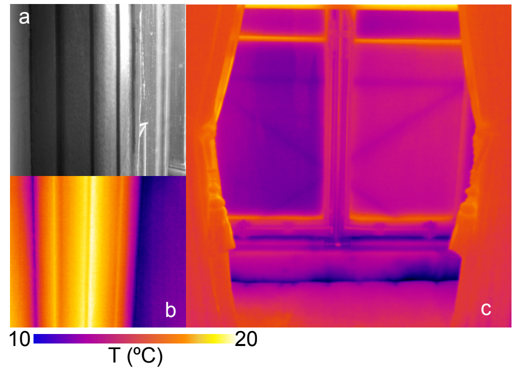

Figure 1: Example of a thermograph of a window. a) and b) show a leak through the window frame.

whereτ is the relaxation time, u_{rms} is the characteristic turbulence root mean square velocity and l is a length scale, taken as the diameter of the particles. For very small values of K_{pt}, we can assume that the turbulent diffusivity of particles is equivalent to the turbulent visco sity of the fluid, i.e. $\varepsilon/\mu_t \simeq 1$. We obtained the range of values of u_{rms} from an steady state simulation. In our case, u_{rms} has an average of $0.0011 \pm 0.0018\ m/s$, with a minimum of $1.83{\times}10^{-7}\ m/s$ and a maximum of 0.043 m/s, and therefore K_{pt} can take values compressed between 10^{-5} and 10^{-2} for our range of particle diameters. The hypothesis is therefore valid.

The second dimensionless number in order of importance is the Péclet number, Pe, which indicates the transport mechanism that dominates the particle flux, i.e. diffusive $Pe < 1$ or convective $Pe > 1$. In our system, as we shall see, we need to deal with some outlet boundaries where the concentration of aerosols is unknown. We can avoid the problem of estimating this concentrations if $1/Pe$ is very small. Fortunately this is the case in our system, where $1/Pe$ = 0.00189 $\pm$ 0.0031, with a minimum of $8{\times}10^{-6}$ and a maximum of 0.12.

EXPERIMENTAL DATA

Particle leakage

We used a thermal camera to locate cracks and leaks in the building envelope. This technique requires a difference of temperature between the indoor and outdoor environments. Consequently, we carried out this survey on a December day (outdoor temperature $\sim$ 8°C), during which the heating system of the house was activated, keeping indoor air at T$\sim$15-20 °C. Under such conditions, air infiltration appeared in the thermal images as a thin line indicating the outdoors temperature. An example is provided in Figure 1.

Our survey revealed that all the detectable leaks were located in the frames and fittings of the windows. The most visible ingress of outdoor air took place from the bottom and top of the windows, in the small gap left between the shutters and the window frame (Figure 1c). This was observed consistently in all the windows. Another typical leaking point is the vertical joint between the two window shutters. This leakage is present in all windows to some degree, generally stretching over 1 m around the handlebar and the bottom of the windows, but in some cases air leaks between the two shutters from top to bottom. These two points of leakage are visible in images of the whole window; however, other leaks require a closer inspection. Close-up images of the window frame revealed the presence of leaks in the fittings between the window frames and the walls. These leaks were also present in all windows over different sections of the window perimeter, typically covering $\sim$ 20-50 % of the total perimeter. We did not detect any cracks in the glass or in the fittings of glass and window frames.

The size of these cracks is not easy to quantify, but they certainly have characteristic dimensions. The depth of a crack can be no larger that the thickness of the window frame, and therefore a representative dimension might be 10 cm. The height of the crack, even on the most visible case of poor fitting of the window shutter in the frame, was significantly smaller than 0.5 cm, and 0.1 cm might be a good estimate of the average cracks found in the house. A particular air entry, a gap under the main gate, deserves separate mention. Its dimensions are greater than those of the average leakage paths, with a height close to 1 cm.

Deposition data

We obtained deposition data from a monitoring campaign carried out by English Heritage in the course of a year, from May 2009 to May 2010 following the method described in [Howell et al., 2002]. Environmental particles were collected in horizontally placed glass slides located at the top of painting frames, at an approximate height of 1.5m. Particles were counted down to 1 μm. A SEM microscope was used to obtain 50 images (in 5 rows of 10) from every sample, and the size of every image was 2×2 mm. The location of the samples reflects the variation of concentration between several rooms and is illustrated in Figure 3. We will refer to every sample by the name of the room. The raw data is in particle counts per 30 days; however, in this work we will use the yearly averages. The experimental values are summarized in Figure 7. In order to enable a comparison with the simulated results, we converted the particle counts into deposition velocities using the following relation:

$$v_{d,exp} = \frac{N}{At}\frac{1}{c} \tag{10}$$

where N is the total particle number, A the area of the surface where the particles were counted, t the elapsed time (a month in seconds), and c is the number concentration of particles surrounding the deposition sampler.

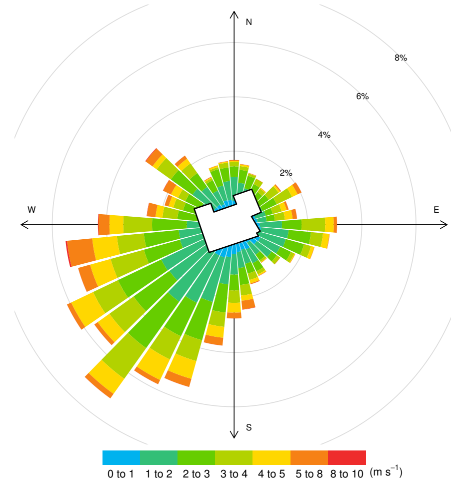

Figure 2: Wind rose showing the orientation of Apsley House.

Naturally, the value of c changes throughout the year. In order to obtain a range of realistic values of $v_{d,exp}$ we shall consider not only the yearly average of c but also its variation. Unfortunately, we do not have direct measurements of the variation of c in Apsley House during the whole period of the experiment, but we do have daily measurements of particle concentration in several rooms and in selected days, which may convey an idea of the typical variability of indoors concentration. The concentration of PM oscillated between 1 and 7.5 μm. This variation is reflected in the box plots of Figure 7.

Air velocities and wind data

We obtained hourly wind data from the MET Office. The closest locations to the site are the Kew and Heathrow weather stations, which display very similar wind roses. Figure 2 shows data from Kew. We assume that wind velocities and directions in Apsley house will not be significantly different.

We used two 3D doppler anemometers to determine indoor velocities and flow patterns. We placed the anemometers in the doors between rooms for periods of 1 h. The observed air directions are in agreement with the CFD simulations. We also used the anemometers to find representative air velocities for the ventilation system.

CFD SIMULATION

Computational model of the building

We produced two computational meshes representing

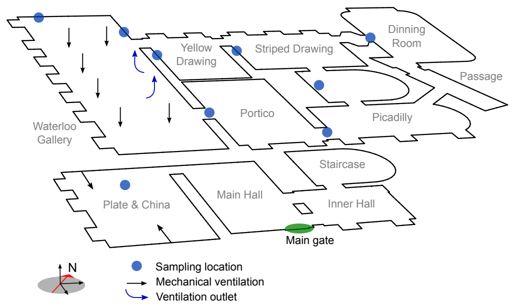

Figure 3: Floor plan of the house with sample locations.

the outdoor and indoor environments. We used a cell size of 1 m in the building surface for the outdoor mesh, and a cell size of 0.3 m for the indoor mesh. Both mesh densities were determined after a grid independence test using the total deposition flux as a test parameter. Both meshes were tetrahedral and unstructured. Figure 3 shows a simplified view of the indoor mesh, with the location of the different rooms and relevant features. Leaks are simplified as a horizontal gap of 10 cm on the top of every window.

Scenario definition

The indoor environment of Apsley House is dominated by a complex combination of different phenomena. Outdoor pollution penetrates mainly through leakage, which is present in all the window frames. Leakage is triggered by the outdoor wind, which can cause a positive or negative pressure on the building walls, thus turning cracks into inlets or outlets of air. Only one of the rooms, the Waterloo gallery, is equipped with an HVAC system that pumps filtered air of outdoor origin into the volume. This system is in continuous operation. The only other room equipped with mechanical ventilation is the Plate and China Room, where two electrical heaters can blow air (of indoor origin) into the room. This system operates intermittently, generally as staff requires, and no record of its operation is maintained. In order to investigate which of these systems has a greater effect on particle deposition, let us artificially divide them in three different modes that can be on and off:

- Mechanical stirring. When this is in place, both the recirculation of the Plate and China Room and the HVAC system in the Waterloo Gallery introduce clean air into the volume.
- Main door. When activated, the gap under the main door allows air to penetrate into the building.
- Leakage. If enabled, the cracks placed on the windows with positive pressure will allow outdoor air to filter with certain penetration factors and air velocities. This option could also be understood as wind on or off.

Table 1: Case definitions for the simulation of Aplsey House. 1 means enabled. The table also indicates if a boundary is considered an outlet (O), an inlet (I) or a wall (W) in each case.

Case	**A**	**B**	**C**	**D**	**E**
Main door	1			1	
Mechanical Stirring		1		1	1
Leakage			1		1
Ventilation outlet	O	O	O	O	O
Waterloo inlets	W	I	W	I	I
Main door	W	W	W	I	I
Positive p walls	W	W	I	W	I
Negative p walls	W	W	O	W	O

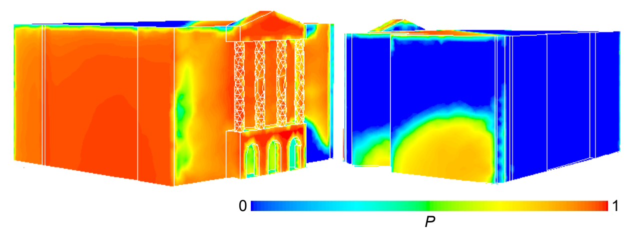

Figure 4: Contours of the penetration factor P on the four faces of Apsley House.

Based on these binary options, we defined six different scenarios (or Cases) which we summarize in Table 1. This cases do not reflect actual operational setups of the house. Rather, they are designed to investigate the relative influence of the different mechanisms that cause deposition, and their synergistic effects.

Particle penetration factors

The simulation of the particle penetration factors provided high values of P in the sides of the house that face the predominant wind directions. There is a clear separation between the South and West façades, where values of P are close to 1 for the most common wind velocities (3 m/s), and the North and East façades, in which the pressure is generally negative and therefore display no particle penetration. Figure 4 clearly reflects this difference.

As Figure 5 shows, there are no significant differences in the value of P between different rooms. When wind speeds are about 0.5 m/s (mild wind, occurrence of $\sim$10%) penetration factors drop significantly. Our simulation indicates that under typical wind conditions, PM of any size up to 10 μm will penetrate efficiently through the building envelope. In mild wind, this penetration is

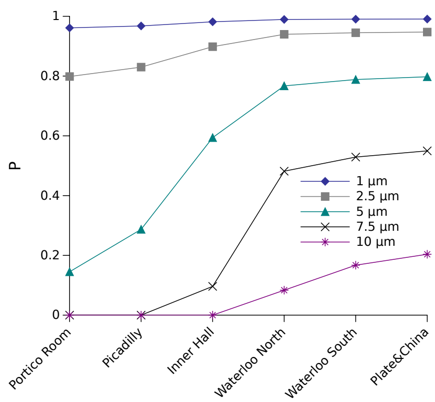

Figure 5: Simulated values of P. Wind speed = 3 m/s, Crack wall roughness, k = 1 μm.

Table 2: Velocity and concentration boundary conditions. u is in m/s.

Boundary	c	u **(max/min)**
China inlets	0.0	(1.5 / 0.5)
Waterloo inlets	0.0	(0.5 / 0.2)
Main door	1	(1 / 0.2)
China leaks	0.90	0.02
Waterloo leaks	0.95	0.02
Piccadilly leaks	0.80	0.02
Portico leaks	0.80	0.02

significantly reduced, and differences in size are less significant.

Given these estimations, we produced a simplified summary of penetration factors and inlet velocities to be used in simulations of the different cases. Table 2 includes this information. We calculated the velocity at the leakage inlets using equation 3

Scenario simulation

We solved the four cases in Fluent for each of the two particle sizes. Particles where characterised with an average diameter of d_p = 2.5 μm with a particle density of ρ_p = 1500 kg/m^3. We normalised the concentration with respect to the outdoor concentration (thus assuming that Aplsey House is immersed in air with a homogenoeous aerosol concentration). Consequently, inlets which are directly connected to the outdoors environment have a concentration of 1, and the leakage inlets have a concentration which is equal to their estimated value of P. The different conditions we set at every boundary are detailed in Table 2. As an example, Figure 6 shows the simulation of case E, where the concentration has been normalised with the concentration in the inlets.

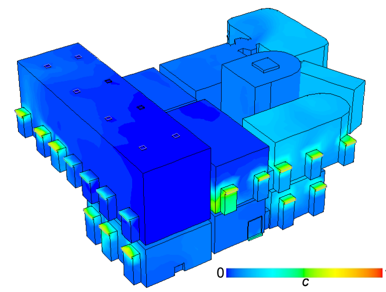

Figure 6: Example of a simulation (case E) whowing computational mesh with contours of normalised concentration (c).

DISCUSSION AND CONCLUSIONS

Figure 7 shows a comparison between the experimentally determined values of v_d and the computational predictions. The most evident result is that the deposition predicted in all cases is within the range of the experimental values. It is also apparent that the effects of the main door alone do not suffice to explain the observed deposition, while leakage and ventilation seem to be accountable for most of the deposition. However, the simulations of these phenomena differ in the prediction of the spatial distribution of deposition. The simulations including forced ventilation can account for the differences in deposition between rooms, but in some cases overpredict the deposition rates. On the other hand, the simulations of leakage underpredict deposition, and do not reproduce the marked differences between rooms.

Interestingly, the deposition that is caused by the ventilation system acting during the whole year corresponds with the maximum measured levels of deposition. This suggests that the introduction in the model of discontinuous or seasonal operation which reflects different operating regimes might reduce this prediction of deposition and bring it closer to the observed yearly averages. A closer inspection of the results reveals that the Dining Room is the only room where deposition is more markedly under-predicted by leakage. This could be related to the fact that this room is equipped with radiators in all its perimeter. Thermal effects can have an impact on deposition that has been ignored in this work, but that should be included in simulations that aim at more precise predictions.

We have shown that a CFD simulation of indoor deposition based on roughly estimated parameters (crack size and number, wind speed and concentration yearly averages), that ignores the yearly variation of some effects (ventilation or heating) and some physical phenomena (heat and coagulation) can deliver fair predictions of overall deposition and its spatial variation. However, our work also demonstrates that more precision can not be

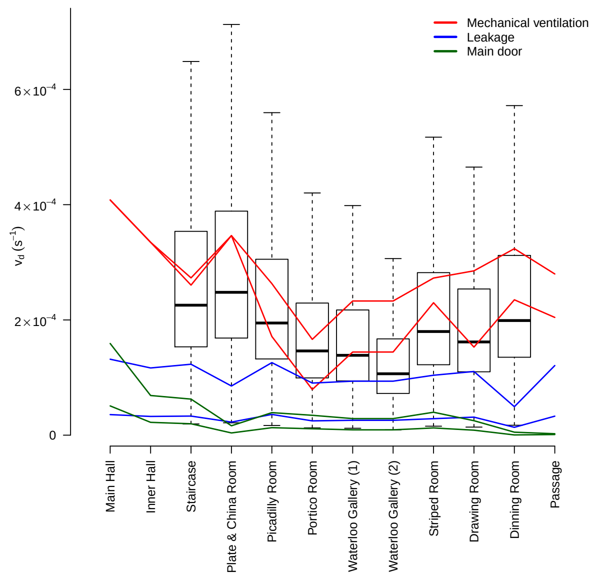

Figure 7: Predicted deposition velocities compared with experimental yearly averages. The continuous lines indicate upper and lower estimations based on the maximum and minimum boundary conditions reported in Table 2 for three different scenarios. The error bars in the experimental values reflect the monthly variation of deposition. We include predictions for some rooms which lack experimental values.

achieved unless the variation of every boundary condition is introduced as an input parameter, and that this variation must be, of course, time-dependent. In other words, seasonal fluctuations must be taken into account if more detail is to be achieved.

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