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CFD Modelling of Air Pollution Dispersion: A UK Urban Perspective

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Abstract - In urban environments, air pollution at the ground level is influenced not only by building configurations but also by roof structures, such as flat, dome, and pitched roofs. The release of pollutants from stacks into the atmosphere plays a significant role in determining air quality. This paper examines the impact of roof configurations on flow dynamics and air pollution dispersion in urban settings. Key parameters, including humidity on the coldest and hottest days of the year in London, as well as wind direction, have been analysed. The results highlight the influence of these factors on air quality. (Wimshurst, n.d.)

***Keywords*:** CFD modelling, urban air quality, street canyon, pollution dispersion, fluid mechanics, building physics

1. Introduction

Air quality is very important in urban complexes since it has several implications for both human safety and the environment. Urban stocks are under strain from urbanisation, which is visible in increased vehicle use and a denser urban fabric. High pedestrian level concentrations are a result of the environment, the city, and the nontrivial combination of pollution sources [1]. In metropolitan settings, transportation and dispersion of pollutants are incredibly challenging.

Vehicle emissions are a significant contributor to the presence of human-made pollution in metropolitan areas. Due to the presence of tall buildings and limited streets in the vicinity, the movement of wind, and the transportation of pollutants in street canyons are more complex due to the shape and structure of the buildings, as opposed to the unobstructed flow of wind over the buildings. Several research studies have been carried out to examine air circulation, the transportation of pollutants, and the mechanisms involved in dilution and removal in street canyons [2].

Numerous prior experimental and numerical investigations have been conducted using idealised representations of building and street configurations, which seldom occur in real-world scenarios. A significant proportion of these studies have specifically assumed uniform flat-roof buildings along the entire street length, as exemplified by the works of [3,4]. However, roofs in the UK are typically constructed with slopes to prevent the accumulation of rainwater and snow. Usually these are stipulated by urban and building planning regulations and include factors such as locally available materials, structural requirements, intended use of the roof space, accessibility, aesthetic architectural considerations, and regional traditions. These elements collectively determine both the shape and pitch of the roof.

This paper aims to develop a numerical model capable of predicting local air quality. The primary objective of this research is to examine the key impacts of domestic and commercial buildings and high-rise structures on air quality, addressing the challenges faced by many boroughs in London. The study focuses on creating a numerical model capable of predicting air pollution at the microscale in urban areas. In this study, the influence of temperature, humidity, and wind velocity on the dispersion and concentration of air pollutants has been investigated. Additionally, the research explores the effects of urban topology, stack shapes, and exhaust velocity on pollutant dispersion and concentration. The initial sections detail the model design, methodology, simulations, results, and evaluation. These are followed by discussions, conclusions, and recommendations for future research.

2. Numerical Model

This study conducted two 2D simulations with ANSYS fluent 2024R1: an isolated flat-roof building with a stack and a configuration of pitched-roof houses typical of the UK, combined with a line source representing vehicle emissions. Vehicle stacks were spaced 0.03 m apart, with the first stack 0.04 m from the last building. Dimensions, scaled 1:200, are detailed in Fig. 1. The computational domain followed Best Practice Guidelines, defined as 5H upstream and laterally and 15H downstream, where H is the height of the tallest building in the domain [5]. Unlike previous studies, this work incorporates temperature, humidity, wind direction, and velocity, based on London's coldest and hottest days in 2023 with data collected from DEFRA, ASHRAE, IQAir, and related organisations. Simulation 1 represents a building with a height of 0.075 m and width of 0.25 m. Simulation 2 involves pitched-roof houses with a height and width of 0.05 m each and a rise-to-run ratio of 0.025:0.025 [6].

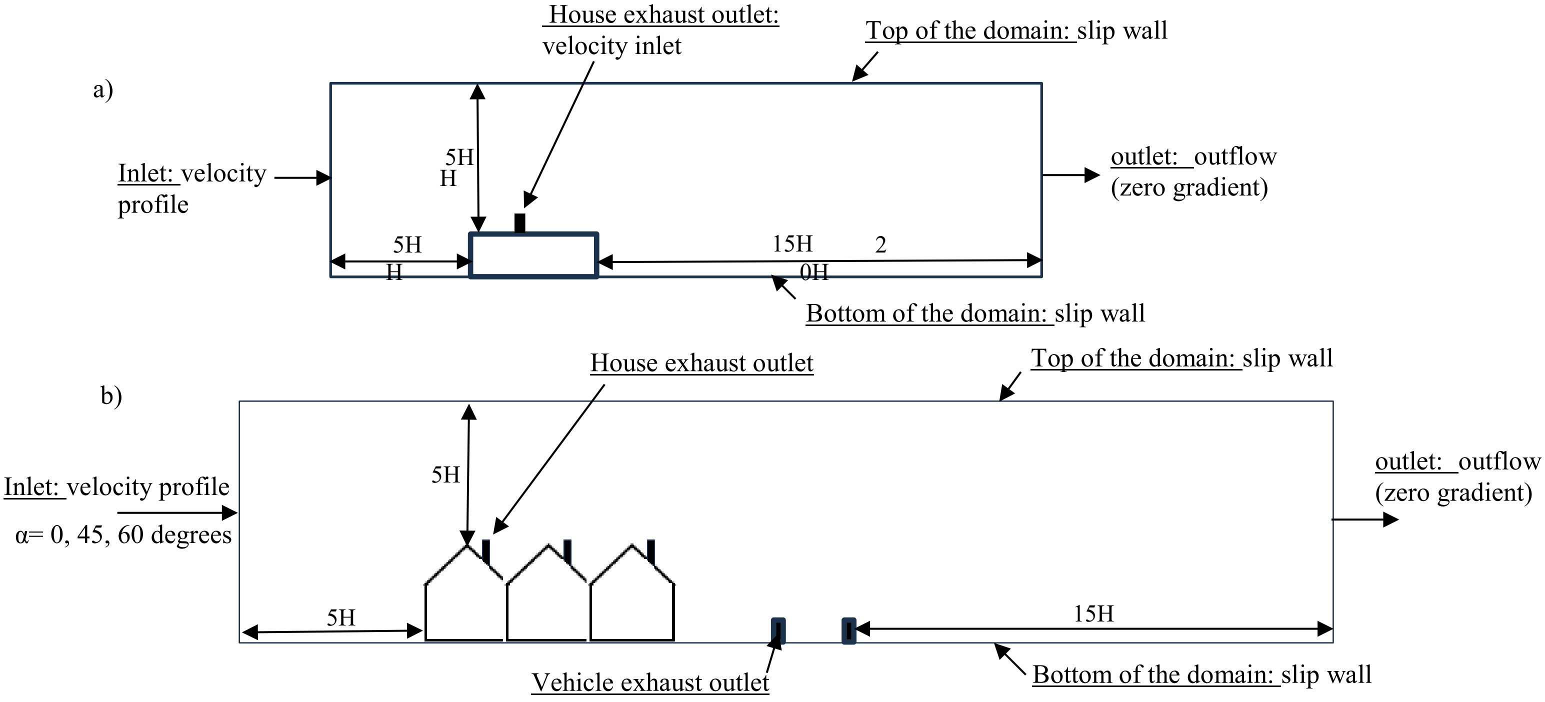

Fig. 1: Schematic Diagram of the Numerical Domain a) Simulation 1, b) Simulation 2

Both simulations were conducted under steady-state, incompressible flow conditions using the realizable k-ε turbulence model with a standard wall function. Pollutant transport was enabled via the species transport option, and the SIMPLE algorithm was employed with residuals set to $1e^{-5}$ and hybrid initialization.

In the first simulation, a wind speed of 6.1 m/s and a stack velocity of 18 m/s (based on $M = v_{wind}/v_{stack}=3$) were used. The species included Sulphur hexafluoride (SF_6) and Nitrogen (N_2) with mass fractions of 0.7 and 0.3, respectively. The temperature was constant at 380 K. Both the building walls and the ground were modelled with no-slip boundary conditions and surface roughness values of K_s=0.0646 [5].

The second simulation analysed winter and summer conditions. For winter, the temperature was set to 277.15 K, humidity to 0.0049 (mass fraction), and wind speed to 5.8 m/s. For summer, the temperature was set to 297.15 K, humidity to 0.0125, and wind speed to 1.0 m/s. The car exhaust velocity was considered as 12m/s and for the houses 4m/s. In both cases, building walls were modelled with smooth brick surfaces (K_s=0.00008) and the ground with asphalt (K_s=0.0003). Pollutant concentrations (PM_{10}, $PM_{2.5}$, NO, and NO_2) are detailed in Table 1 and are considered inert for the purpose of this investigation.

Table 1: Boundary Conditions for the Second Simulation a) Winter, b) Summer.

a)

Pollutants	**Cars**	**Houses**
PM_{10}	0.00114	0.0062
$PM_{2.5}$	0.00071	0.00453
NO	0.0022	0.00059
NO_2	0.00229	0.00104

b)

Pollutants	**Cars**	**Houses**
PM_{10}	0.00075	0.000393
$PM_{2.5}$	0.000385	0.000263
NO	0.00092	0.00014
NO_2	0.001455	0.00054

2.1. Model Pre-processing and Numerical Validation

Reynolds numbers calculated for both case studies confirmed turbulent flow, and inflation layers with face meshing were applied. Using ANSYS Fluent Mesh, 6 mesh sizes were created for the first simulation, and a grid independence test was performed by measuring velocity through the domain. Fig. 2 presents the mesh statistics, and the validation graph. The minimal velocity differences (less than 4%) across meshes confirm mesh independence. The final mesh resolution of 0.002 m element size was selected for optimal accuracy. The second simulation setup was developed using the validated first model.

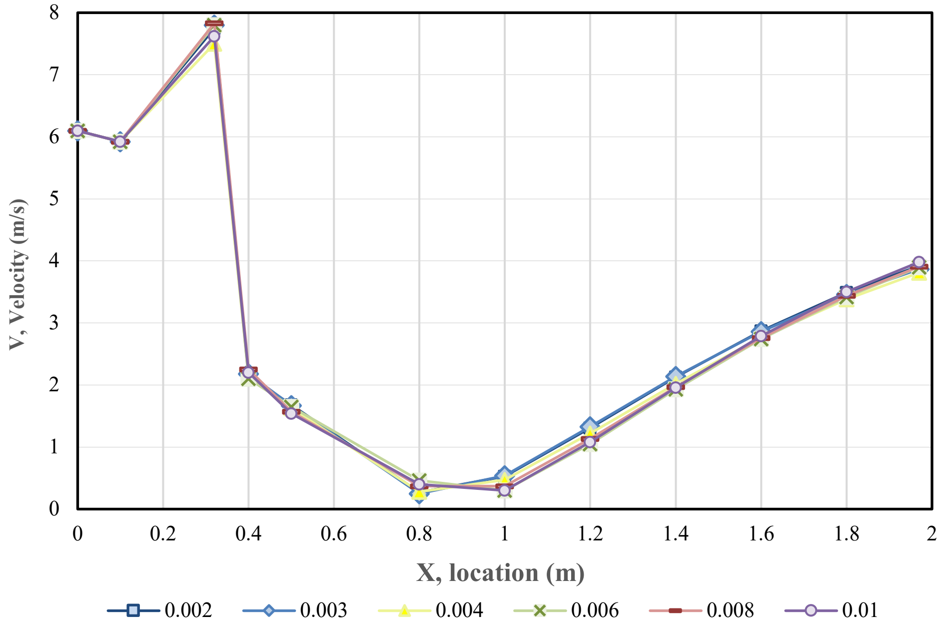

Fig. 2: Numerical Validation and Grid Independency Test Results [5].

3. Results and Discussion

Fig. 3 (a) presents the CFD simulation results for the velocity field of the first case. The results illustrate a decrease in wind velocity on the leeward wall, leading to the formation of a recirculation zone characterised by a sharp velocity gradient. Fig. 3 (b) illustrates the dispersion characteristics of N_2, highlighting its accumulation and mixing within the recirculation wake region located behind the building.

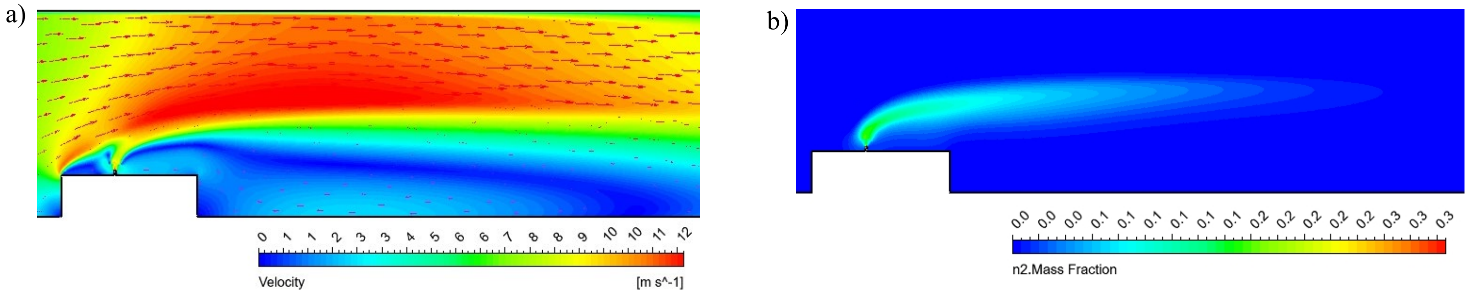

Fig. 3: a) Velocity Distribution Around the Building, b) Nitrogen Mass Fraction Contour [5].

Fig. 4 compares velocity contours for pitched-roof houses and vehicle emission stacks under wind directions of 0, 45°, and 60°, respectively. In Fig. 4 (a), with a wind direction of 0°, the lack of angular deviation minimises turbulence, resulting in a more uniform velocity distribution downstream. The Fig. 4 (b) illustrates the dispersion of PM2.5, showing higher concentrations near the emission source and a gradual decrease downstream. The distribution highlights the influence of wind flow on pollutant dispersion and accumulation in the wake region behind the buildings. At 45°, Fig 4 (c), pronounced recirculation zones and strong turbulence form behind the buildings, creating low-velocity regions conducive to pollutant accumulation. In contrast, the 60° wind, Fig. 4 (d) results in smoother airflow, with less intense recirculation and more uniform downstream velocity. This comparison highlights the influence of wind direction, with oblique angles (60°) reducing turbulence and improving flow uniformity compared to steeper angles (45°).

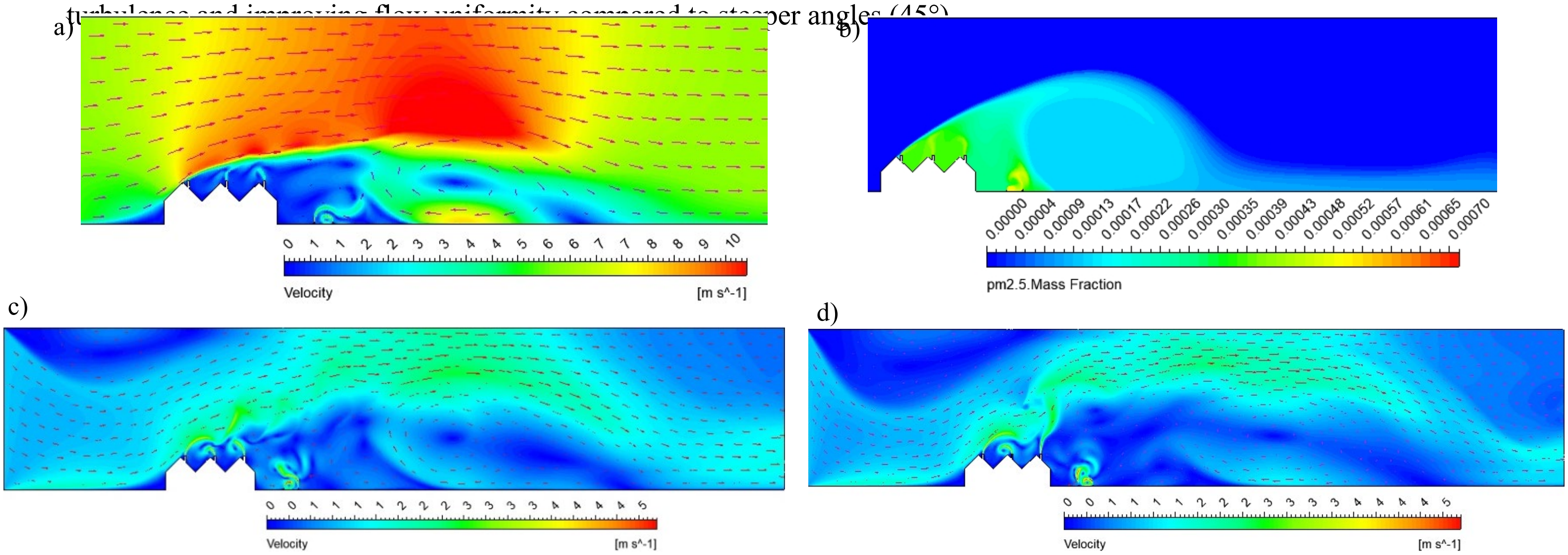

Fig. 4: a) Velocity Distribution With 0 Angle, b) $PM_{2.5}$ Mass Fraction Contour in the Winter With 60° Wind Velocity, c) Velocity Distribution With 45° Angle, d) Velocity Distribution With 60° Angle

4. Conclusion

This study conducted a numerical analysis of a street canyon to evaluate the impact of roof configurations and wind direction on flow dynamics and pollutant dispersion. The findings revealed that pitched roof designs consistently reduce wind velocity and turbulence, leading to decreased ventilation efficiency. Additionally, the simulations highlighted the formation of vortices in the leeward side and between buildings. Understanding the location and characteristics of these vortices is crucial for improving knowledge of pollutant dispersion in urban environments and informing strategies for better air quality management.

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