City Scale Pollutant Dispersion Modelling Utilising a Combination of Computational Fluid Dynamics and Standard Air Quality Simulation

Neihad Hussen Al-Khalidy[1]

***Abstract*—** Pollutant dispersion in urban street canyons is usually investigated numerically using Standard Air Quality (AQ) modelling assessment, ie through the application of validated 3-D computer modelling tools such as CALPUFF or Advanced Computational Fluid Dynamic (CFD) for near-field Simulation. This paper presents a road map to use a combination of 3-D standard air quality modelling and Computational Fluid Dynamics (CFD) to reliably simulate air flow and quality in city canyons on the example of emergency ventilation smoke control in roadway tunnels. The local wind rose for a project site was created using The Air Pollution Model (TAPM) and CALMET diagnostic meteorological modelling software, which reconstructs local 3D wind and temperature fields starting from regional meteorological measurements, synoptic weather model outputs, topography and land use data. Emissions from the project site have then been initially modelled using the CALPUFF dispersion model. Boundary conditions (the worst case wind direction, wind speed and ambient temperature) resulting in the highest pollutant concentration predictions were identified through this preliminary CALPUFF dispersion modelling study, which were then used in the detailed microclimate CFD exhaust dispersion modelling. Microclimate CFD modelling is substantially more computationally expensive than preliminary CALPUF simulations. The CFD analysis offers a comprehensive range of output including pollutant concentration, velocity distribution, temperature distribution, pressure profile, turbulent levels, etc. allowing the identification of sources that have unacceptable impact on the city air quality. Downwind pollutant concentrations can be further reduced by optimising the stack dimensions and/or smoke volumes and speeds. It is anticipated that the use of CFD for entire city modelling will be a useful tool to help urban designers and environmental planners. The paper also discusses some of the challenges facing CFD for modelling built environment.

***Keywords*—** CFD, Pollutant Dispersion, Wind, Emergency Ventilation Smoke, Transportation Tunnel.

I. INTRODUCTION

In order to maintain a healthy environment it is essential to be able to predict, evaluate and understand airflow patterns and dispersion of pollutants within populated areas.

Far-field pollutant dispersion is usually investigated numerically using "Standard" operational air quality - assessment, ie through the application of validated 3-D computer modelling tools such as Gaussian models (CALPUFF, Aeropol, Aermode, etc) and Lagrangian/Eulerian Models (GRAL, TAPM, etc). Standard dispersion modelling uses mathematical modelling of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere.

Many of these models such as CALPUFF and TAPM are used for regulatory purposes [1, 2].

Different types of dispersion models are overviewed and outlined in [1] to [6]. Many of the Gaussian models have been shown to over predict concentrations in low wind speed condition [3]. In general, those models are not recommended for areas heavily influenced by turbulence such as in an urban environment due to turbulence modelling approximation [6].

Predicting air and pollutant in an urban environment is a very complex problem influenced by downwash and acceleration effects induced by surrounding buildings. Recently, the use of numerical techniques including Computational Fluid Dynamics (CFD) to simulate pollutant distribution and wind patterns caused by building configurations has received much attention. CFD can be used as a tool to help the designer to examine the pollutant problem under various conditions.

A considerable number of CFD publications have been published in the Journal of Wind Engineering & Industrial Aerodynamics in the past two decades. CFD predictions of wind flow around bluff bodies have been compared and validated against wind tunnel and full scale measurements in the open literature [ie 7, 8, and 9]. In general good agreement is obtained when best practice guidelines are used for the modelling.

A CFD simulation of airflow and pollutant dispersion around a group of real buildings configuration is presented in [10]. The need for that study was a result of a city council requirement prior to the issue of a construction certificate for a proposed building. The pollutant sources were located on the roof of the building. Results of the simulation were presented for near calm and windy conditions. The compliance with Occupational Health and Safety Commission (OHSC) requirements is also demonstrated in that study.

The dispersion of gases from diesel/gas powered electricity generators within and then downstream of building complexes in the entire inner Brisbane city was presented in [11]. That

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study accounted for effect of buildings geometry, upwind buildings configuration, canyon orientation, wind speed, wind direction and pollutant sources are accounted for.

In this study, a combination of standard air quality dispersion modelling and advanced Computational Fluid Dynamics (CFD) assessment was used to reliably assess the dispersion characteristics in city canyons. The main objectives of this study are to:

1) Develop a 3D CAD model of building complexes for CFD dispersion modelling.
2) Incorporates the emission sources into the model.
3) Develop localised weather data for the project site.
4) Develop procedures to integrate data from the standard (Mesoscale metrological) model into the CFD microclimate numerical model.
5) Predict pollutant concentrations on the ground and facades of buildings where intakes of air conditioning systems are located.
6) Provide recommendations to improve air quality of the project pollutant sources.

II. Problem Formulation

The data of interest in this study are the **maximum 1-hour average** concentrations of pollutant, eg CO, PM10 and NOX ($\mu g/m^3$) experienced at the surrounding buildings during an emergency fire event in a transportation tunnel.

Preliminary modelling of emissions from a project site has been performed using a combination of the TAPM, CALMET and CALPUFF models. CALPUFF is a transport and dispersion model that ejects “puffs” of material emitted from modelled sources, simulating dispersion and transformation processes along the way. In doing so it typically uses the fields generated by a meteorological pre-processor CALMET, discussed further below in Section 3. The CALPUFF dispersion model has the ability to handle calm wind speeds and complicated terrain and was considered appropriate for the prediction of the worst case wind conditions for microclimate pollutant dispersion analysis. The objective of this preliminary modelling was to identify the worst case meteorological conditions that give rise to the worst-case downwind concentrations, which were then used in the detailed CFD exhaust dispersion modelling.

A detailed Computational Fluid Dynamic (CFD) pollutant simulation was then used to quantify pollutant dispersion on the ground level and on the façades of the nearby buildings under the identified worst case meteorological conditions.

The CFD model solves the continuity, momentum, energy and species concentration equations. The equations for a steady state case can be written as follows:

$$\frac{\partial}{\partial x_i}(\rho\, u_i) = 0$$

$$\frac{\partial}{\partial x_j}(\rho\, u_i\, u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}) + \rho\, g_i + F_i$$

$$\frac{\partial}{\partial x_i}(\rho\, h) + \frac{\partial}{\partial x_i}(u_i\, \rho\, h) = \frac{\partial}{\partial x_i}(k_{effective}\frac{\partial T}{\partial x_i}) + S$$

$$\frac{\partial}{\partial x_j}(C u_i) = \frac{\partial}{\partial x_i}(\frac{v_t}{\sigma}\frac{\partial C}{\partial x_j})$$

Where ρ is the density, u is the velocity, p is the static pressure, ρg and F are the gravitational body and external body forces, ι_{ij} is the stress tensor, h is the enthalpy and $k_{effective}$ is the effective thermal conductivity, C is the pollutant concentration and v is the kinematic viscosity and S is the volumetric heat source.

Turbulence is predicted using one of the following methods:

- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- Reynolds-Averaged Navier-Stokes (RANS) Equations

For most real world building problems turbulence is, in principle, described by the Navier-Stokes equations [12]. Commercial CFD codes provides a wide range of turbulence models including Spalart-Allmaras model, k-epsilon (ke) models, k-w models, v2f model, Reynolds Stress models, Scale Adaptive Simulation (SAS) model, Detached Eddy Simulation, Large eddy simulation (LES) models. The quality of CFD simulation depends on the selected turbulence model. In practical problems the turbulence model should be as simple as the relevant physics will permit

III. Case Study – Emergency Tunnel Ventilation

The design fire parameters used for the design of tunnel emergency ventilation have a significant impact on the tunnel design and users safety. In order to improve the safety of transportation tunnels, it is essential to be able to predict, evaluate and understand airflow patterns and dispersion of pollutants within populated areas during fire events and emergency tunnel ventilation.

The flow patterns that develop around buildings govern the distribution of pressure and consequently the concentration distribution of pollutants in a built environment. Given the complexity of built environments, the dispersion of pollutants resulting from a city scale project will be complex, influenced by downwash and acceleration effects induced by surrounding buildings, wind tunnelling through the aligned open areas, the location of the source point, ambient meteorological conditions, etc.

Pollutant dispersion is therefore a function of the following parameters:

1) Upstream wind characteristics: wind speed and direction, turbulence intensity, etc.
2) Stack position relative to surrounding buildings, stack height, exit velocity and temperature.
3) Surrounding building configuration, both upwind and downwind.
4) Interaction of flow patterns associated with adjacent

buildings.

This study provides a roadmap to optimise the design of emergency tunnel ventilation utilising advanced numerical techniques. The proposed methodology involved the followings:

1) Obtain or predict the wind rose for the project site. In this study the TAPM prognostic model [13], developed by the Commonwealth Scientific and Industrial Research Organisation (CSIRO) was used to generate the upper air data required for CALMET modelling. TAPM predicts wind speed and direction, temperature, pressure, water vapour, cloud, rain water and turbulence. The program allows the user to generate synthetic observations by referencing databases (covering terrain, vegetation and soil type, sea surface temperature and synoptic scale meteorological analyses) which are subsequently used in the model input to generate one full year of hourly meteorological observations at user-defined levels within the atmosphere. Additionally, the TAPM model may assimilate actual local wind observations so that they can optionally be included in a model solution. The wind speed and direction observations are used to realign the predicted solution towards the observation values. However, for this study no data assimilation has been used to nudge (i.e. influence) the TAPM predictions and the model was instead run without any observational data assimilation. TAPM generated three dimensional meteorological data was used as the initial guess wind field for a CALMET meteorological model that develops hourly wind and other meteorological fields on a three-dimensional gridded modelling domain that are required as inputs to the CALPUFF dispersion model. CALMET modelling was conducted using the nested CALMET approach, where the final results from a coarse-grid run were used as the initial guess of a fine-grid run. This has the advantage that off-domain terrain features including slope flows, blocking effect are allowed to take effect and the larger –scale wind flow provides a better start in the fine-grid run. Associated two dimensional fields such as mixing height, surface characteristics and dispersion properties are also included in the file produced by CALMET. The interpolated wind field is then modified within the model to account for the influences of topography, sea breeze, as well as differential heating and surface roughness associated with different land uses across the modelling domain. These modifications are applied to the winds at each grid point to develop a final wind field. The final hourly varying wind field thus reflects the influences of local topography and land uses.
2) Hourly surface meteorological data from Bureau of Meteorology (BOM) stations located near the project site were incorporated in the CALMET modelling. The output from the outer domain CALMET modelling was then used as the initial guess field for the inner domain CALMET modelling. The computational domain encompassed an area of 6 km × 6 km. A horizontal grid spacing of 0.1 km was used to adequately represent the important local terrain features and land use. A summary of the annual wind behavior predicted by CALMET for the project site for one calendar year is presented in Figure 1.

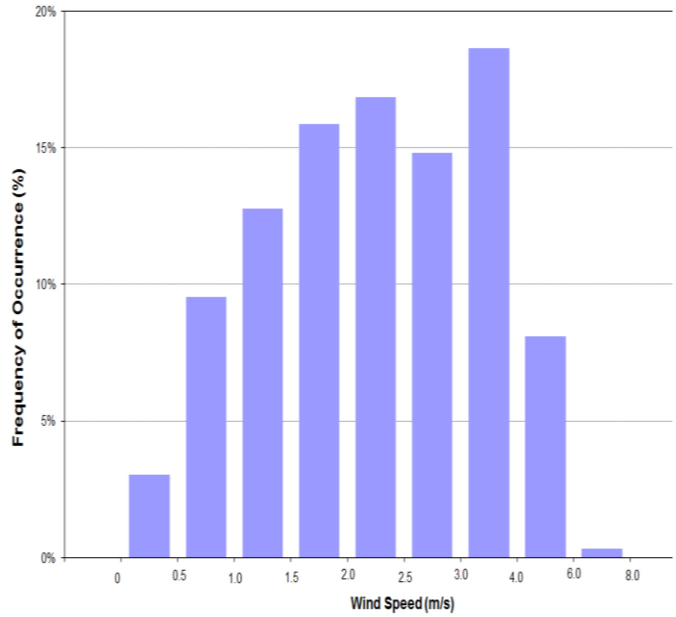


Fig.1 G Wind speed Frequency Distribution for the Project Site, as predicted by CALMET for one Calendar Year

1) Conduct a preliminary CALPUFF atmospheric dispersion modelling. Boundary conditions (eg the worst case wind direction, wind speed and ambient temperature) resulting in the highest pollutant concentration predictions were identified through this preliminary CALPUFF dispersion modelling study, which were then used in the detailed microclimate CFD exhaust dispersion modelling.
2) Develop a detailed 3D CAD model of the proposed project site for CFD modelling.
3) Incorporate the emergency ventilation shafts (stacks) into the model.
4) Add topography and surrounding buildings to a minimum radius of 500 m.
5) Develop mixed meshed cells (tetrahedral, hexahedra and pyramids) or polyhedral mesh for the computational domain.
6) Integrate the previously predicted local weather data for the worst case scenarios with the developed CFD model. In this case number of runs for microclimate CFD runs is significantly reduced. It is important to understand that microclimate CFD modelling is substantially more computationally expensive than preliminary CALPUF simulations.
7) Establish the emission rates for pollutant (CO, PM10, etc.) at the ventilation shafts. Data are obtained from the fire model for the project.
8) Calculate initial turbulence quantities (kinetic energy and dissipation rate) required for the upwind free boundary from empirical relationships.
9) Select a proper turbulence model and numerical scheme for the assessment based on available best practice guidelines and/or validated studies.

10) Predict pollutants concentration (or dilution factors) and assess the Emergency Ventilation Smoke (EVS) impact of the project site on surrounding buildings and infrastructure.
11) Provide guidance as to the areas where adopted pollutants acceptability criterion had the potential to be exceeded and an indication as to the likely local optimum treatment strategy.
12) In consultation with the project team revise the design where required by optimising the stack location, dimensions and/or smoke volumes and speeds.

The above procedure allows assessing design modification options including all parameters of interest (Building configuration, detailed stack geometry and position, topography, etc.) in a timely manner.

A. Modelling Configuration

A 3D model of the project site and surrounding buildings and structure blocks was created from the architectural drawings and CAD models supplied by the client. The 3D model of the stacks and surrounding blocks is shown in Figure 2. The CFD model incorporated the following:

1) A calculation domain of 2,000 m length, 2,000 m wide and 500 m high was used for the CFD analysis.
2) Four rail tunnel stacks with three stacks are operated simultaneously as per the proposed design.
3) Accurate terrain effect of the modelled area.

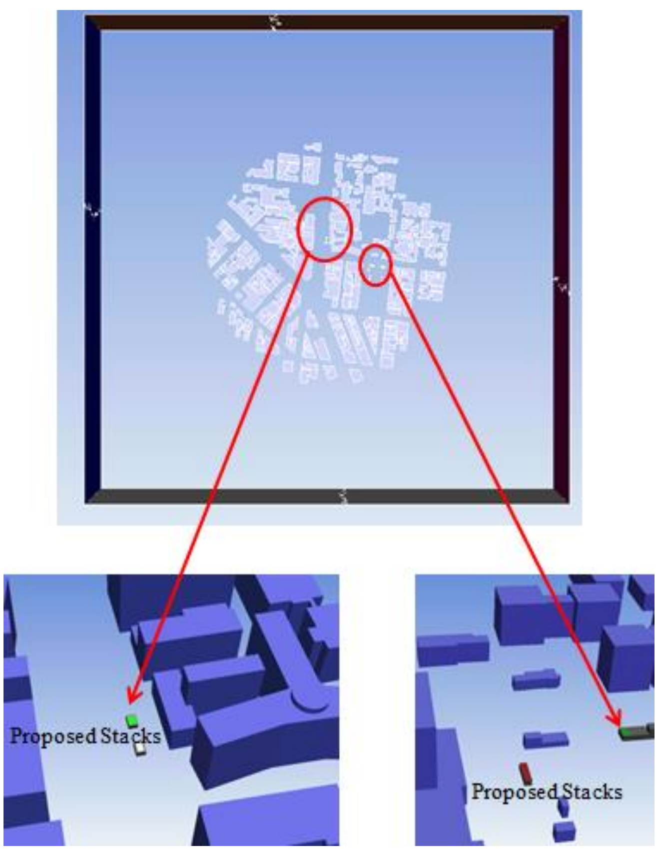


Fig.2 Geometry for CFD Modelling

B. Discretization

The software package utilised in the current CFD analysis is the commercially available code ANSYS-Fluent [14]. The CFD model solves continuity, momentum, energy and species equations in the computational domain to predict the steady state airflow and pollutants dispersion at and around the project site.

1) The quality of the mesh is a critical aspect of the overall numerical simulation and it has a significant impact on the accuracy of the results and solver run time. For the current analysis, polyhedral elements with a total number of 14,212,493 nodes were used to cover the computational domain (Refer Figure 3). Polyhedral cells are especially beneficial for handling complex flows and used to provide more accurate results than even hexahedra mesh. For a hexahedral cell, there are three optimal flow directions which lead to the maximum accuracy while for a polyhedron with 12 faces; there are six optimal directions which together with large number of neighbors lead to a more accurate solution with a lower cell count.
2) The following techniques were used for discretization:
   - A second order numerical scheme for discretization of pressure to obtain more accurate results.
   - A second order numerical scheme for discretization of momentum to obtain more accurate results.
3) A Realizable k-epsilon (rke) turbulence model was used for all analysed cases due to ability to handle recirculation, high gradients and computational time advantages.
4) The solution is combined with a wall function to avoid using very fine elements near the wall.
5) An iterative procedure was used to estimate the air velocity in terms of three directions, pollutants concentration, pressure profile and turbulence parameters.

The normalised residuals of continuity for all cases were reduced by at least three orders of magnitude while the normalised residual of x-, y-, and z-velocity, species, temperature, k and epsilon was reduced between four and six orders of magnitude demonstrating a valid solution (Refer Figure 4).

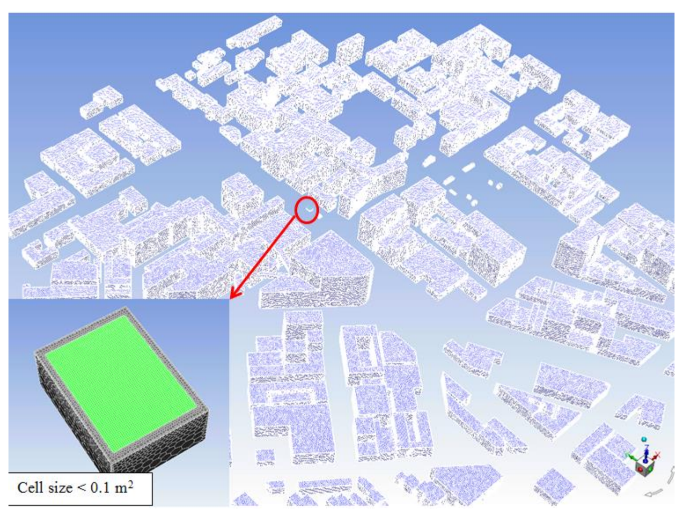


Fig.3 Polyhedral Mesh

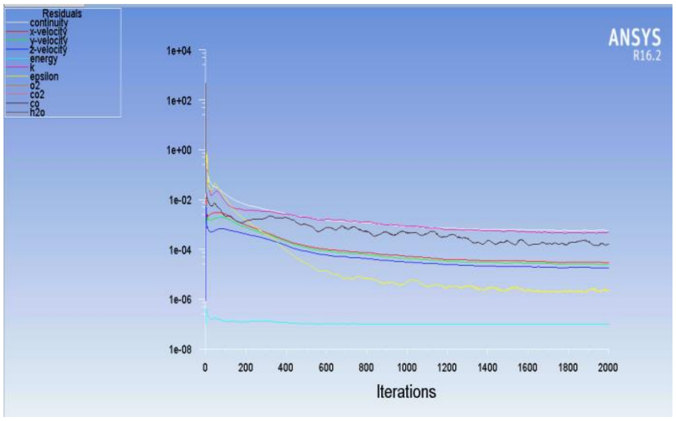


Fig. 4 Scaled Residual History

C. CFD Results and Discussion

In the wind and pollutant dispersion CFD modelling, wind speed and pollutant concentration can be reported at any point on the ground, podium and at any vertical elevations. The area of interest therefore includes all surrounding buildings shown in Figure 2. Results of simulations in Figure 5 to Figure 13 are presented for the following worst case atmospheric condition:

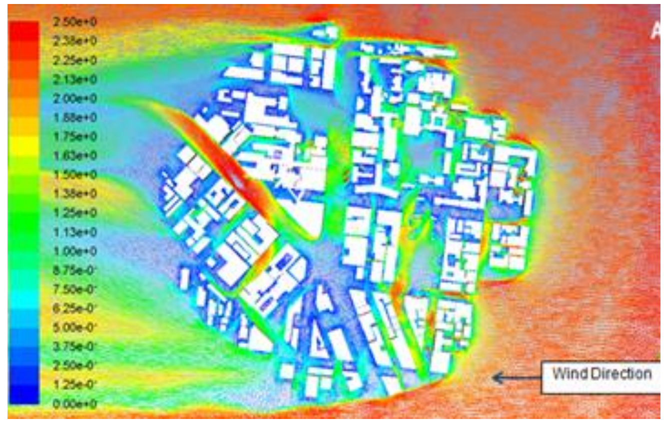
Wind Speed = 2.30 m/s
Wind Angle = 92°
Ambient Temperature = 299.3K.

Lower temperature exhaust gas emissions data are related to small fire sizes. The highest exhaust gas temperature at the inlet to the central fans located closest to the fire found through literature research was163˚C for a 100 MW fire and 107˚C for a 20 MW fire [15]. In this study small and large fire sizes are considered. Results in Figure 5 to Figure 13 are for a smoke (exhaust) temperature of 315 K (15 degrees above ambient temperature).

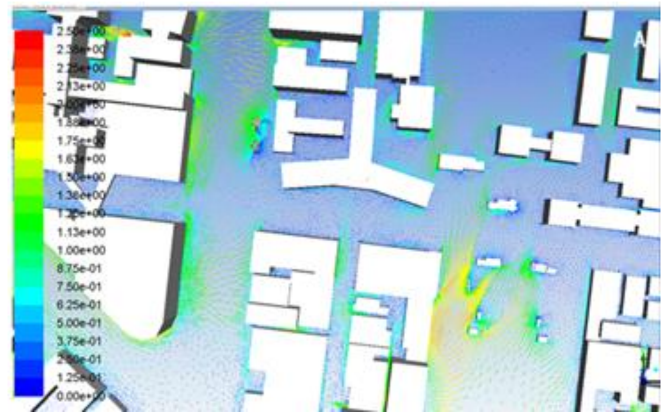
Exhaust speed of 5 m/s is proposed and was applied to all modelled stacks. A pollutant concentration of unity was assumed at the sources and dilution factors are predicted in the areas of interest.

Figure 5 shows the vectors of mean airflow velocities through a two-dimensional section above the ground of the project site. Velocity vectors are plotted on a colour coded scale between 0 and 2.5 m/s. Dark blue represents still conditions at 0 m/s and red representing the strongest wind speed. The following conclusions can be reached from Figure 5:

1) General flow characteristics for the modelled built environment are shown in Figure 5A. The CFD model captures the fluid flow characteristics in significant detail. Wind is approaching the site from the east with a wind speed of 2.3 m/s as per the given boundary conditions. Wind is then accelerated near the edges and stagnated and recirculated behind the buildings.
2) The stacks receive some shielding from the upstream buildings (Refer Figure 5B).



A: General Flow Characteristic



B: Flow at the Stack Locations

Fig.5 (A & B) Velocity Vector Coloured by Velocity Magnitude (m/s)

The velocity vectors at the stack exits are shown in Figure 6. One can see that the smoke speed is 5 m/s at the operated stacks (three in total) as per the given boundary conditions.

The pollutant dispersion has been analysed on the ground level and at the faces of the surrounding buildings where the intakes of air conditioning systems are located and shown in Figure 7 to Figure 9. The concentration profile and dilution factor are plotted on a colour coded scale between 0 - 0.0006 and 0 - 0.003 respectively. Dark blue represents zero concentration and red representing the highest concentration.

The maximum concentration of pollutant, eg CO and NOX (µg/m3) experienced at the ground and surrounding buildings can be calculated by multiplying the predicted Dilution Factor by the pollutant concentration (µg/m^3) at the sources. The following can be concluded from the above figures:

1) The concentration profile and dilution factor are plotted on a colour coded scale between 0 - 0.0006 and 0 - 0.003 respectively. Dark blue represents zero concentration and red representing the highest concentration.
2) The maximum concentration of pollutant, eg CO and NOX (µg/m^3) experienced at the ground and surrounding buildings can be calculated by multiplying the predicted Dilution Factor by the pollutant concentration (µg/m3) at the sources. The following can be concluded from the above figures:

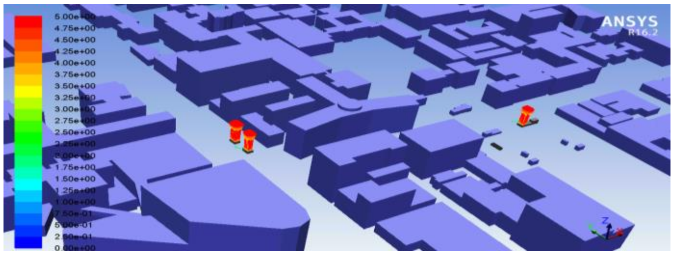
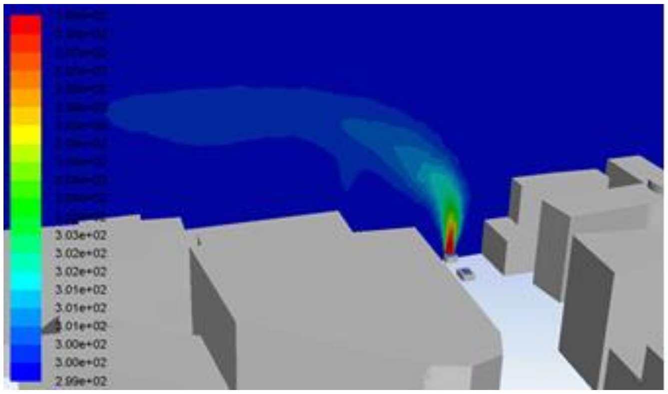
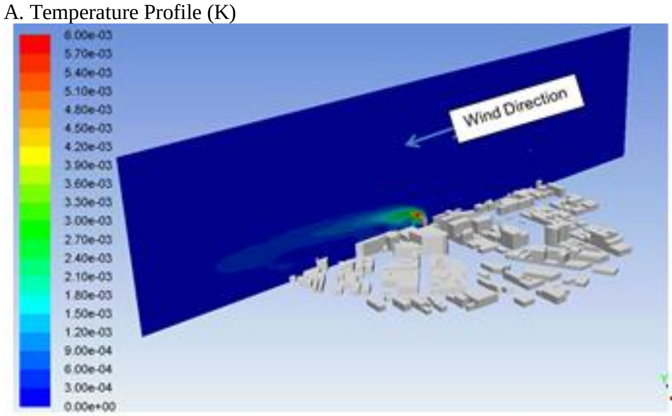


Fig.6 Velocity Vector (m/s) at the smoke Sources



A. Temperature Profile (K)



B. Concentration Profile (Dilution Factor)

Fig.7 (A & B) CFD Results at Selected 2D Vertical Section through one of the Exhaust Shafts

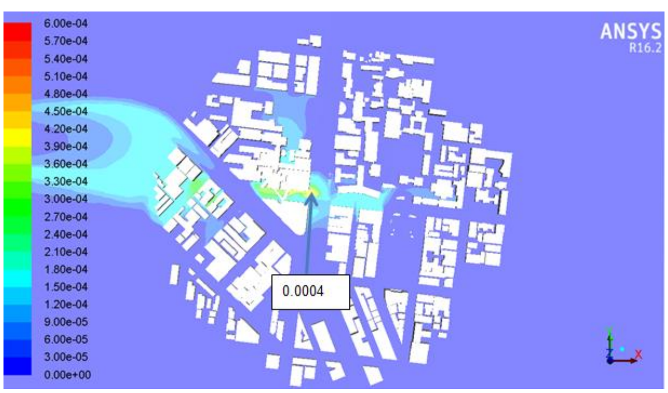


Fig.8 Concentration Profile (Dilution Factor) on the Ground Level

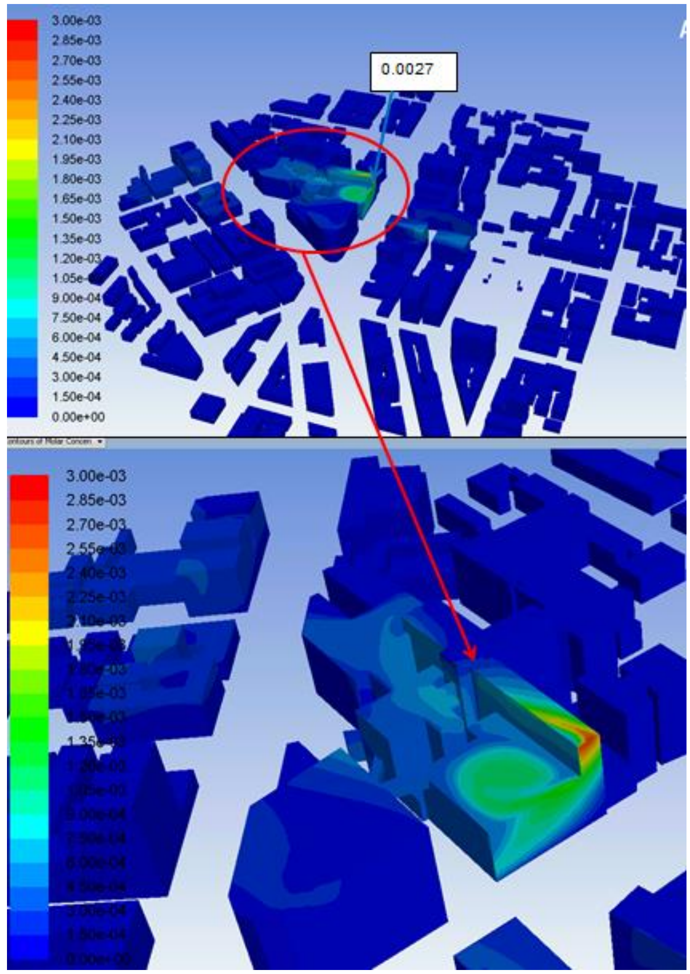


Fig.9 Concentration Profile (Dilution Factor) on the Facades of Buildings

A fume iso-surface indicating the approximate spread of pollutants with a downwind concentration of 0.01 times the initial exhaust concentration or higher in three-dimensions is also shown in Figure 10.

The spread of pollutants with downwind concentrations between 0.005 and 0.002 times the source concentration are presented in Figure 11 to Figure 13.

A fume concentration distribution at each ventilation shaft is determined from the fire model for the project. Pollutant concentrations on the ground and facades of buildings are calculated using the predicted dilution factors and then compared against the assessment criteria.

The study accounted for other worst case scenarios and assessed various fire sizes.

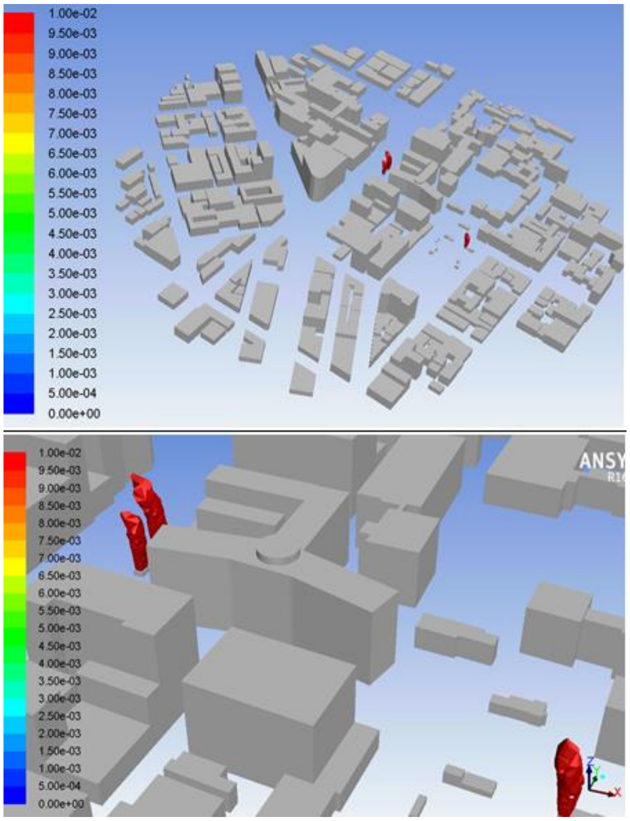


Fig.10 Concentration Profile (Iso Surface of 0.01 Dilution Factor)

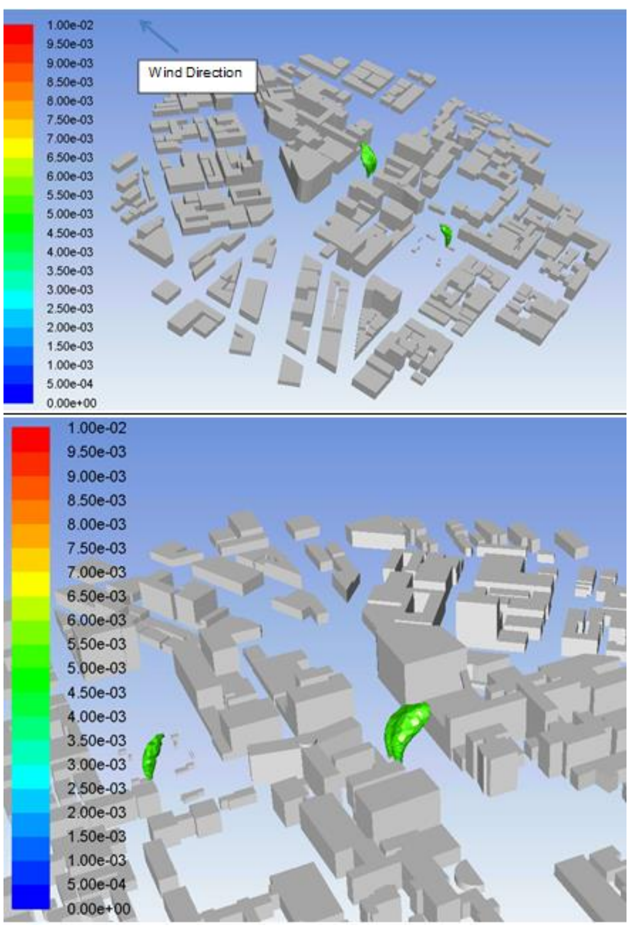


Fig.11 Concentration Profile (Iso surface of 0.005 Dilution Factor)

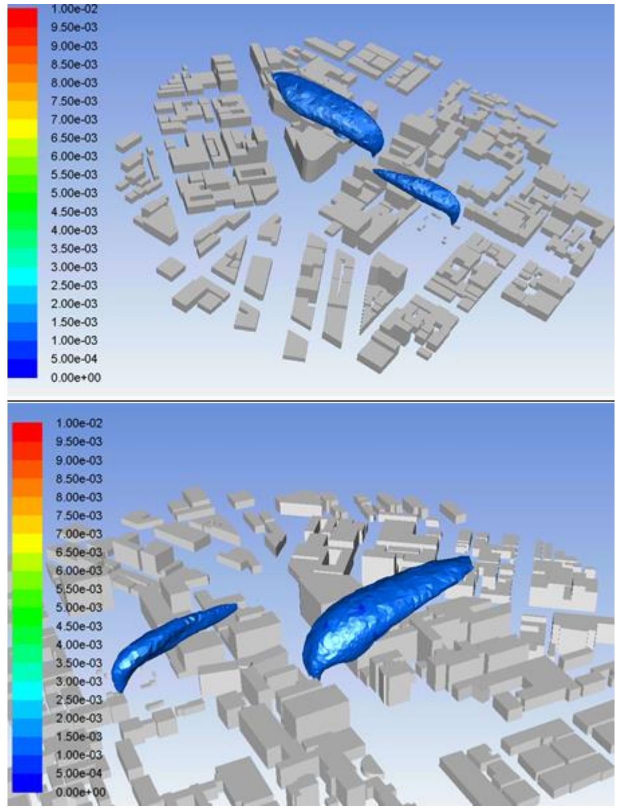


Fig.12 Concentration Profile (Iso Surface of 0.001 Dilution Factor)

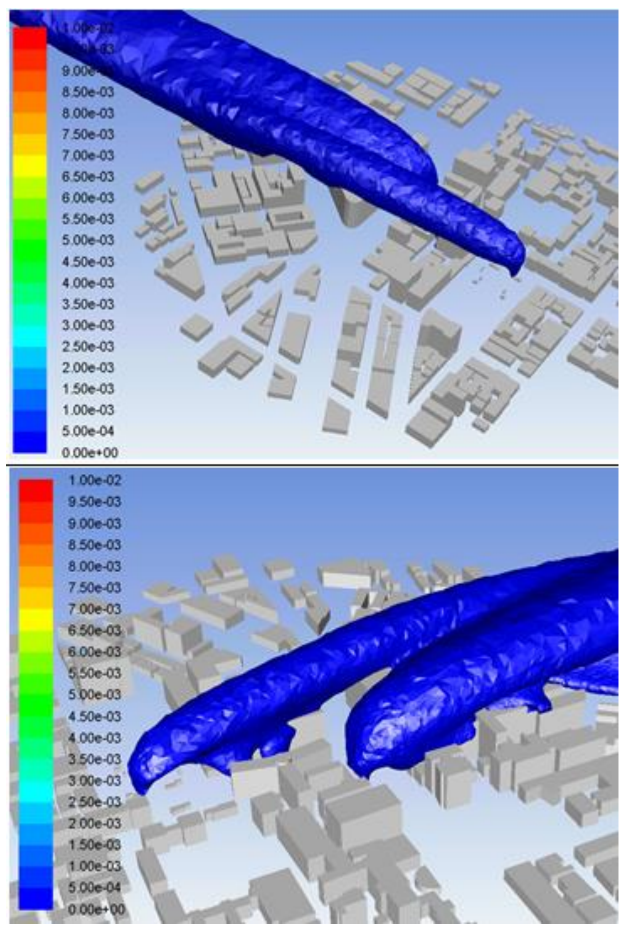


Fig.13 Concentration Profile (Iso Surface of 0.001 Dilution Factor)

IV. CONCLUSION

This paper presents a road map to use a combination of 3-D standard air quality modelling and advanced Computation Fluid Dynamics (CFD) to reliably simulate air flow and quality in city canyons on the example of emergency ventilation smoke control in roadway tunnels. The local wind rose for the project site was created using The Air Pollution Model (TAPM) and CALMET diagnostic meteorological modelling software. Emissions from a project site have then been initially modelled using the CALPUFF dispersion model. Boundary conditions (eg the worst case wind direction, wind speed and ambient temperature) resulting in the highest pollutant concentration predictions were identified through this preliminary CALPUFF dispersion modelling study, which were then used in the detailed microclimate CFD exhaust dispersion modelling. The CFD analysis offers a comprehensive range of output including pollutant concentration at any point on the ground, podium and at any elevations, velocity distribution, temperature distribution, pressure profile, turbulent levels, etc. allowing the identification of sources that have unacceptable impact on the city air quality. It is anticipated that the use of CFD for entire city modelling will be a useful tool to help urban designers and environmental planners. The paper also discusses some of the challenges facing CFD for modelling built environment.

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