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## **A numerical analysis of pollutant dispersion in street canyon: influence of the turbulent Schmidt number**

**Key words:** pollutant dispersion, urban street canyons, build configurations, CFD simulation turbulent Schmidt number

### **Introduction**

Several approaches have been conducted over the past decades to study the flow field, pollutant dispersion and deposition inside urban street canyons. These investigations include physical modeling, CFD and full-scale measurements of the wind flow and scalars dispersion within and above the urban canopies. A detailed reviews of the modeling techniques for flow fields and pollutant transport within street canyons is presented by Vardoulakis, Fisher, Pericleous and Gonzales-Flesca (2003), Ahmad Khare and Chaudhry (2005), Li, Liu, Leung and Lam (2006) and recently Tominaga and Stathopoulos presented in 2013 an overview of CFD modeling procedures used to study wind and pollutant transport in the urban environment.

Physical modeling involves simulation of airflow and pollutant dispersion using wind-tunnel (Rafailidis & Schatzmann, 1995; Meroney, Rafailidis & Pavageau 1996; Meroney, Leidl & Rafailidis, 1999, Pavageau & Schatzmann, 1999; Kastner-Klein & Plate, 1999; Baker & Hargreaves, 2001; Kovar et al., 2002, Gromke & Ruck, 2007) water channel (Baik & Kim 2000; Caton, Britter & Dalziel, 2003; Kim & Baik, 2005; Li, Leung, Liu & Lam, 2008), where flow can be controlled, and complex urban morphology can be simulated in fine details, i.e. including facades, arbitrary roof shape, trees and other street furniture. Also, the results obtained from this approach are generally used to validate numerical models.

Rafailidis and Schatzmann (1995) proposed and investigated experimentally at the Meteorological Institute of Hamburg University, several idealized 2D building configurations, under a simulation of toxic emissions from ve-

hicle exhaust in street canyons. In their experiments, in a quasi-two-dimensional setup, multiple street-canyon configurations with a variety of canyon aspect ratios,  $B/H$ , and roof shapes were placed in a simulated deep urban boundary layer. A tracer gas was emitted by a line source placed at the bottom of one street canyon and the concentrations of pollutant were measured at several locations on the walls and roofs of buildings on either side of the street containing the source (Fig. 1), and it is presented in dimensionless form  $K(K = CUHL/Q)$ , where  $C$  [vol·vol] denotes the tracer concentration,  $U$  [ $\text{m}\cdot\text{s}^{-1}$ ] is the free stream velocity,  $H$  [m] is the building height,  $L$  [m] is the length of the line source and  $Q$  [ $\text{vol}\cdot\text{s}^{-1}$ ] the source strength.

Due to increasing computer power, numerous studies using CFD techniques have been performed using RANS models and lately LES, DES and DNS approaches, simulating explicitly detailed flow, pollutant dispersion patterns in street canyons related to various param-

eters such as street geometries, building roof shapes, thermal effects and trees planting (Sini, Anquetin & Mestayer, 1996; Rafailidis, 1997; Theodoridis & Moussiopoulos, 2000; Xiaomin, Zhen & Jiasong, 2005; Xie, Huang & Wang, 2005; Nazridoust & Ahmadi, 2006; Huang, Hu & Zeng, 2009; Yassin, 2011; Salim, Buccolieri, Chan & Di Sabatino, 2011; Gallagher, Gill & McNabola, 2012; Tong & Leung, 2012; Moonen, Gromke & Dorer, 2013; Takano & Moonen, 2013; Allegrini, Dorer & Carmeliet, 2014; Cui, Li & Tao, 2014; Liu & Wong, 2014; Madalozzo, Braun, Awruch & Morsch, 2014; Ng & Chau, 2014; Efthimiou, Berbekar, Harms, Bartzis & Lietl, 2015). Some of these CFD studies have been performed to investigate in detail the effects of building configuration on flows and pollutant dispersion. These studies often employ simple building configuration to study how the geometry and different roof shapes can affect airflow and pollutant fields in a 2D idealized street canyons (Theodoridis & Moussiopoulos,

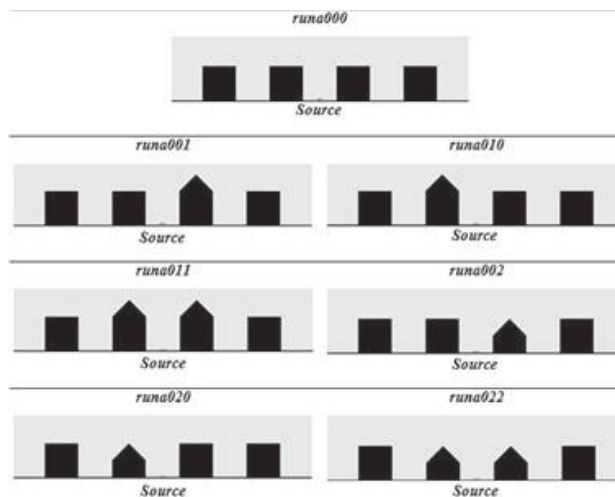


FIGURE 1. Definition of the street canyon configuration cases

2000; Chan, Dong, Leung, Cheung & Hung, 2002; Assimakopoulos, ApSimon & Moussiopoulos, 2003; Xiaomin, Zhen & Jiasong, 2005; Nazridoust & Ahmadi, 2006; Huang, Jin & Sun, 2007; Huang, Hu & Zeng, 2009; Yassin, 2011; Takano & Moonen, 2013). The most commonly RANS turbulent models used in street canyon simulations are the standard  $k-\varepsilon$  model, renormalization group *RNG*  $k-\varepsilon$  model and realizable  $k-\varepsilon$  model and their performance are tested in some of the studies. The turbulent Schmidt number which is defined as the ratio between the rate of turbulent transport of momentum and the turbulent transport of mass is introduced in the pollutant transport equation.

parameter that depend on the mean flow, turbulence fields and the spatial patterns of pollutant in street canyons (Koeltzsch, 2000; Blocken, Stathopoulos, Saathoff & Wang, 2008; Tominaga and Stathopoulos, 2013). Moreover, great importance in Air Quality Modeling within Urban street canyons is the specification of a suitable turbulent Schmidt. The values of  $Sc_t$ , the turbulence models and CFD codes used in several numerical investigations are summarized with the corresponding authors in Table 1. At the first glance, it sounds that the choice of the turbulent Schmidt number value is arbitrary.

Our purpose throughout the work is to establish the link between a specific

TABLE 1. Several CFD studies for the pollutant dispersion in street canyons using turbulence approach

| Author(s)            | CFD code          | Turbulence approach                     | Turbulence Schmidt number |
|----------------------|-------------------|---|---------------------------|
| Sini et al. (1996)   | CHENSI            | RANS – $k-\varepsilon$ model            | 0.9                       |
| Baik et al. (2000)   | in-house CFD code | RANS – $k-\varepsilon$ model            | 0.9                       |
| Huang et al. (2000)  | in-house CFD code | RANS – $k-\varepsilon$                  | 0.5                       |
| Yassin et al. (2011) | fluent            | RANS – $k-\varepsilon$                  | 0.9                       |
| Baik et al. (2002)   | in-house CFD code | RANS – $k-\varepsilon$ model            | 0.9                       |
| Gromke et al. (2009) | fluent            | RANS – $k-\varepsilon$ model            | 0.6                       |
| Huang et al. (2009)  | fluent            | RANS – $k-\varepsilon$ model            | 0.7                       |
| Takano et al. (2013) | OpenFOAM          | RANS – $k-\varepsilon$ model            | 0.3                       |
| Huang et al. (2015)  | fluent            | RANS – $k-\varepsilon$ model            | 0.7                       |
| Gromke et al. (2015) | fluent            | RANS – realizable $k-\varepsilon$ model | 0.5                       |

The ability of CFD models to predict accurately pollutant dispersion in urban areas depends on the turbulent Schmidt number value, which has an important implication on measurement of pollution concentration field (Flesch, Prueger & Hatfield, 2002). The turbulent Schmidt number  $Sc_t$  is a fitting

application on building configurations; in the real case; and the equilibrium of the mass turbulent transport types, which may be achieved by the turbulent Schmidt number, in order to approach the experimental solutions. Several values of  $Sc_t$ , are applied for finding the most suitable number to be associated. Particular at-

attention is paid to the effect of the turbulent Schmidt number, since this possibility has not yet been explored. Numerical simulations are conducted in that sense.

## Material and methods

The computational investigations are performed using the CFD-code ANSYS CFX (ANSYS Academic Research, Release 16.2). In all simulations, the flow field is calculated using Reynolds Averaged Navier Stokes (RANS) with the standard  $k-\varepsilon$  (Launder and Spalding, 1974) and  $RNG\ k-\varepsilon$  (Yakhot et al., 1992) turbulence models. For modeling the pollutant dispersion, the additional variable transport equation (Eq. 1) is solved using the mean velocity field from the  $k-\varepsilon$  and  $RNG\ k-\varepsilon$  models, and with a turbulent Schmidt number varying from 0.1 to 1.3.

$$\frac{\partial(\rho C)}{\partial t} + \frac{\partial}{\partial x_j}(\rho U_j C) = \frac{\partial}{\partial x_j} \left[ \left( \rho D_C + \frac{\mu_t}{Sc_t} \right) \frac{\partial C}{\partial x_j} \right] \quad (1)$$

where:

$C$  – pollutant mean concentration;

$Sc_t, \mu_t$  – the turbulence Schmidt number and the turbulence viscosity;

$D_C$  – the molecular diffusivity coefficient of the pollutant.

## Computational domain and grid generation

In order to verify the influence of the turbulent Schmidt number on numerical predictions of pollutants dispersion in street canyons, seven geometrical configurations are defined as indicated in Figure 1 by considering the case

where  $B/H = 1$  as reference configuration (case runa000), where  $B$  is the street canyon width  $B = 0.06$  m), and  $H$  is the building height  $H = 0.06$  m. All cases (Fig. 2) considered in this investigation have been studied experimentally by Rafailidis and Schatzmann (1995). The data sets of these experiments are accessible to the researchers with interest in validation of numerical micro-scale dispersion models and can be found online at [http://www.mi.uni-hamburg.de/fileadmin/files/static\\_html/windtunnel](http://www.mi.uni-hamburg.de/fileadmin/files/static_html/windtunnel), and an additional detailed descriptions and measurements of the wind tunnel experiments is given by Rafailidis (1995).

For all cases, five street canyons are considered in the computational domain. The street canyon with the pollution source is the third one away from the inflow boundary, which is surrounded by the buildings (upwind or downwind) that do not usually have the same rectangular geometry. As the wind is orthogonal to the direction of the streets and assuming that the length of the street canyon is infinitely long, the computational domain is simplified from a three-dimensional domain to a two-dimensional frame.

The 2D computational domains have been created and meshed with the ANSYS ICEM software. In Figure 3 we defined the numerical domain configuration adopted in these numerical simulations. The domain dimensions are  $11 H \times 10 H$  in the x- and z-directions, respectively. A multi-block topology strategy is used to build a mesh for all geometry cases. The multi-block structure gives more flexibility in the design of their mesh so that the highest mesh quality can be achieved. Trial runs with different meshes are performed to ensure

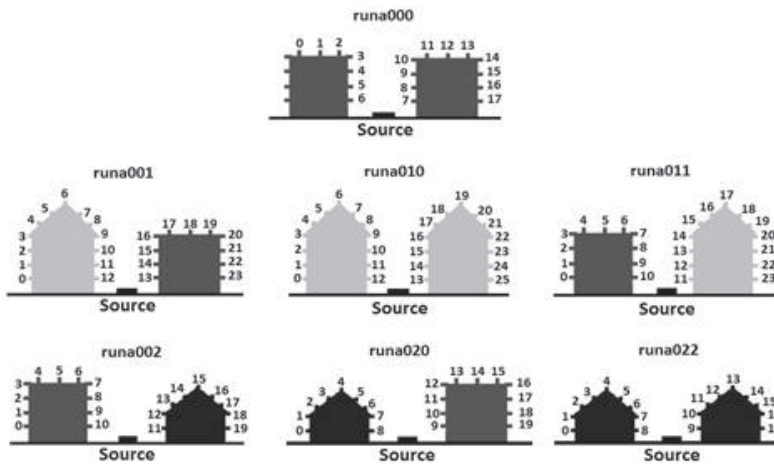


FIGURE 2. Positions of measurements on the building faces and roofs

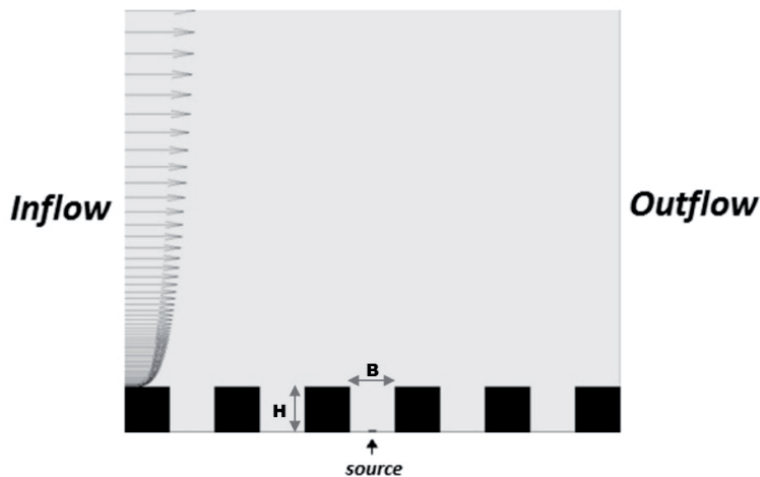


FIGURE 3. Schematic diagram of the computational domain for a street canyon,  $B/H = 1$

that the CFD model is independent from mesh size before a final mesh is selected. The total number of generated cells is about 25–40,000 elements with  $30 \times 30$  cells are placed in each street canyon as recommended by Franke, Hellsten, Schlünzen and Carissimo (2007). In the streets, the minimum cell size is of  $1 \times 1$  mm (applied on the building surfaces and the grounds) increasing gradually to a maximum of  $25 \times 25$  mm (at the

middle of street). In the vertical direction, away from the roofs of buildings, the cell size is increased gradually by an inflation ratio of mesh kept between 1.033 and 1.11 to a maximum of 30 mm at the top of the domain.

### Boundary conditions

In all cases simulated in this investigation, identical boundary conditions for airflow and pollutant are imposed as fol-

lows: At the inflow boundary, the measured distributions of longitudinal wind velocity  $U(z)$  and the turbulent intensity  $I(\%)$  are used. This information is obtained from the vertical profiles of  $U(z)$  and  $I(\%)$  measured above the street canyon with pollutant source (Rafailidis, 1997). The turbulence kinetic energy and dissipation are estimated as  $k_{inlet} = \frac{3}{2} I^2 U^2(z)$  and  $\varepsilon = k^{3/2} \cdot l_t^{-1}$ ,

where  $l_t$  is the eddy length scale, chosen as approximately  $H$ . Over the outlet of computational domain, the relative static pressure is specified as its default value of zero. At the upper surface of computational domain, a free-slip boundary condition is imposed and the pollutant mass flux to the surface is assumed to be zero. The boundary conditions used at the entrance of the pollution source are exactly the same parameters as those of the experiment conducted at the Meteorological Institute of Hamburg University (Rafailidis, 1995). The pollutant considered is in the form of a mixture of ethane ( $Q_{C_2H_6} = 4 \text{ l}\cdot\text{h}^{-1}$ ) and air ( $Q_{Air} = 100 \text{ l}\cdot\text{h}^{-1}$ ). A turbulence intensity of 1% has been used as boundary condition at the inlet of the pollutant in the street canyon with pollutant source, and at all solid walls, the no-slip boundary condition is applied.

## Results and discussion

In this study, the numerical simulations are done for seven different geometries of building shape roofs around the street with pollutant source. All cases were investigated by two turbulence models,  $k-\varepsilon$  and *RNG*  $k-\varepsilon$ , and each case was systematically investigated by changing the turbulent Schmidt number

varying from 0.1 and 1.3. The wind direction orientation was normal to the longitudinal axis of the studied street canyons. The velocity fields were solved for wind velocity of  $5 \text{ m}\cdot\text{s}^{-1}$  taken from the experiment measurements at reference height of 0.5 m above ground level. The pollutant is emitted from steady line source located at the center of the ground level in the street canyon of interest which represents the third street in the numerical domain, and is modeled as a passive scalar.

In this section, the CFD results of the mean velocity, and pollutant dispersion in street canyon are presented. These computed results are compared with experimental measurements of Rafailidis and Schatzmann (1995), and the recommended turbulent Schmidt number for each geometry configuration of street canyon is validated with the experimental data. The influence of the turbulent Schmidt number on pollutant passive scalar predictions is discussed.

Streamlines of mean velocity fields obtained from the numerical simulations of all cases (runa000 to runa022) are shown in Figure 4. As can be established, the shape of the roofs is the most important parameter making the air velocity field. The airflow pattern in street canyon with pollutant source is strongly influenced by the roof shapes of the upstream and downstream building. Predicted velocity fields have shown that the two turbulence models,  $k-\varepsilon$  and *RNG*  $k-\varepsilon$ , give very similar air velocity fields.

In all cases, the flow field is generally controlled by one large vortex formed inside the street canyon. However, the vortex shape, circulation and location of its centre differ for each case. These dif-



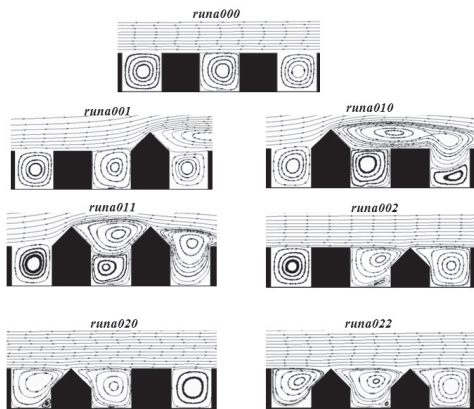


FIGURE 4. Streamlines in street canyon, obtained with the standard model, for all cases

ferences produce different velocity contours and consequently a significant influence on pollutant distribution in street canyon.

### Flow field in street canyons

In Figure 4, we present the flow fields inside street canyons using streamlines. For the runa000 configuration only one main vortex, rotating clockwise, is formed at the centre of the street canyon. A similar vortex structure is found in case runa001 configuration of street canyon, but the main vortex is distorted and shifted towards the downstream building side. In the cases runa010 and runa011, a specific recirculation in the region near the roofs can be found for each configuration due to the influence of the edge of the leeward building on the flow separation above the street. In both cases, two main vortices are formed, with the upper one rotating clockwise above the canyon and the lower one rotating counter-clockwise inside the canyon. The main vortex is shifted and distorted upwards towards the roof of the downstream building.

Moreover, a formation of a weak secondary vortex is observed near the source at the lower downstream building corner with the opposite rotation to the main vortex. In the street canyon of cases runa020, runa020 an runa022, one main vortex in the middle of the canyon is formed and distorted along the inclined roof of the upstream building.

In the cases runa002 and runa022, it can be observed that the main vortex center is shifted upward in the street canyon compared with cases run020, and the main vortex is distorted along the inclined roofs of the upstream building for runa020 and of the upstream and downstream building for runa022. The formation of a small vortex at the lower downstream building corner of the street canyon has been also noticed.

### Analysis of dimensionless pollutant concentrations

In Figure 5, we present a comparison between calculated dimensionless pollutant concentrations  $K$  for all cases obtained by both  $k-\varepsilon$  and  $RNG k-\varepsilon$  turbulence models for various turbulent Schmidt number varying from 0.1 to 1.3, and measured values along the upstream and downstream building roofs and sides as reported by Rafailidis and Schatzmann (1995). To avoid cluttering the graphs only results from minimum and maximum values of  $Sc_t$  are reported (Fig. 5). Calculated dimensionless pollutant concentrations  $K$  are close to the experimental values measured along the upstream and downstream building roofs and the building sides of canyons adjacent to street with pollutant source. Both  $k-\varepsilon$  and  $RNG k-\varepsilon$  models give approximately the same tendency. However, it

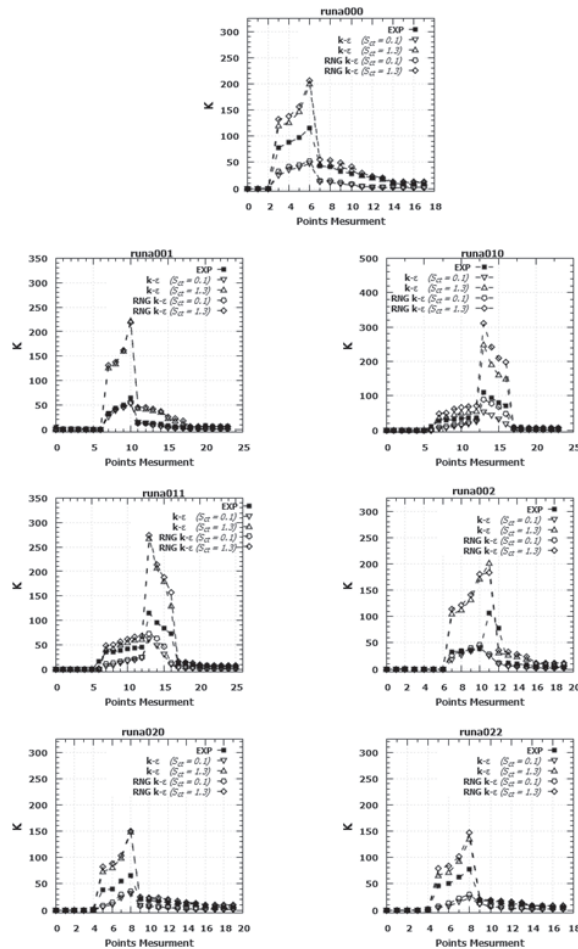


FIGURE 5. Dimensionless concentration  $K$ -distributions for all cases

can be seen that  $RNG\ k-\epsilon$  model gives higher concentration than the  $k-\epsilon$  model for a same turbulent Schmidt number. It can be also noted that  $Sc_t$  has significant influence on the predicted concentration levels especially the distribution of dimensionless concentration measured on the sides of the buildings in the canyon with pollutant source. This influence is observed while changing the Schmidt number in the same numerical model. As  $Sc_t$  increases, calculated dimensionless pollutant concentrations  $K$  increases

on both side of the street with source for both and turbulence models in all cases.

### Analysis of appropriate $Sc_t$ number

The sum of the relative errors (SER) is used to determine the appropriate  $Sc_t$  number for each case. It is defined as the sum of the magnitude of the difference between the experimental and the simulation values of the dimensionless concentration  $K$  divided by the sum of the experimental values of  $K$  as follows:



$$SRE = \frac{\sum_1^n |K_{i,Exp} - K_{i,Sim}|}{\sum_1^n K_{i,Exp}} \quad (3)$$

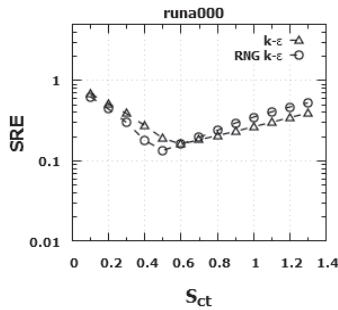


FIGURE 6. Sum of the relative errors for reference case runa000 calculated for both and turbulent models

In Figure 6, we show a comparison of the relative error calculated for reference configuration (runa000). It can be seen that the appropriate turbulent Schmidt number corresponding to the minimum error obtained using  $k-\epsilon$  model is 0.6 and it is 0.5 when using  $RNG k-\epsilon$  turbulence model.

The results presented in Figure 7 show different appropriate Schmidt number found for all configurations investigated regardless of the turbulence model used in the numerical approach. We can notice a significant differences in appropriate Schmidt number value when changing the configuration of the street

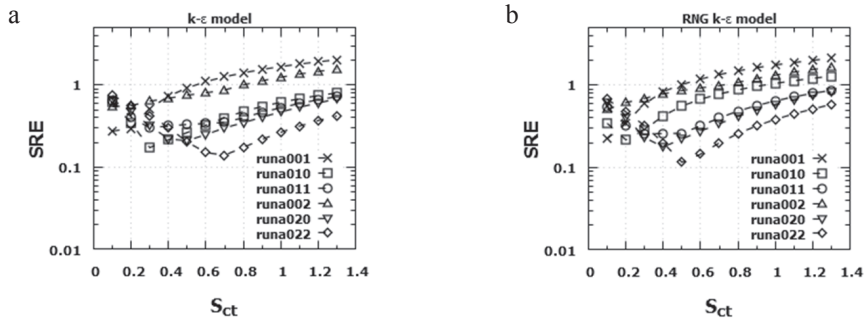


FIGURE 7. Sum of the relative errors for cases: runa001, runa010, runa011, runa002, runa020, runa022: calculated for  $k-\epsilon$  turbulent model (a), calculated for  $RNG k-\epsilon$  turbulent model (b)

TABLE 2. Appropriate  $Sc_t$  number for different canyon geometries and turbulence models

| Turbulence model | Case    |         |         |         |         |         |         |
|------------------|---------|---------|---------|---------|---------|---------|---------|
|                  | runa000 | runa001 | runa010 | runa011 | runa002 | runa020 | runa022 |
| $k-\epsilon$     | 0.6     | 0.1     | 0.3     | 0.3     | 0.1     | 0.5     | 0.7     |
| $RNG k-\epsilon$ | 0.5     | 0.1     | 0.2     | 0.3     | 0.1     | 0.4     | 0.5     |

The sum of relative errors are calculated for all cases for both  $k-\epsilon$  and  $RNG k-\epsilon$  turbulent models, and are determined from the measurement points of leeward and windward sides.

canyon. It can also be observed that the appropriate Schmidt values corresponding to the model  $k-\epsilon$  and the model  $RNG k-\epsilon$  are almost identical. For all cases, appropriate  $Sc_t$  values varied between

0.1 and 0.7 for  $k-\epsilon$  model and between 0.1 and 0.5 for  $RNG k-\epsilon$  model.

In Table 2, we summarize the results of the appropriate turbulent Schmidt number corresponding to the minimum error. The results reported in Table 2 show that the appropriate  $Sc_t$  number is strongly dependent on the turbulence model and on the street canyon geometrical configuration.

In Figure 8, a comparison of the experimental and simulation results for all cases for both  $k-\epsilon$  and  $RNG k-\epsilon$  turbulence models is presented. The profiles in the Figure 8 give dimensionless concentration  $K$  comparison between numerical results calculated with appropriate  $Sc_t$  and experimental results of Rafailidis and Schatzmann (1995). It is found that turbulent Schmidt number provid-

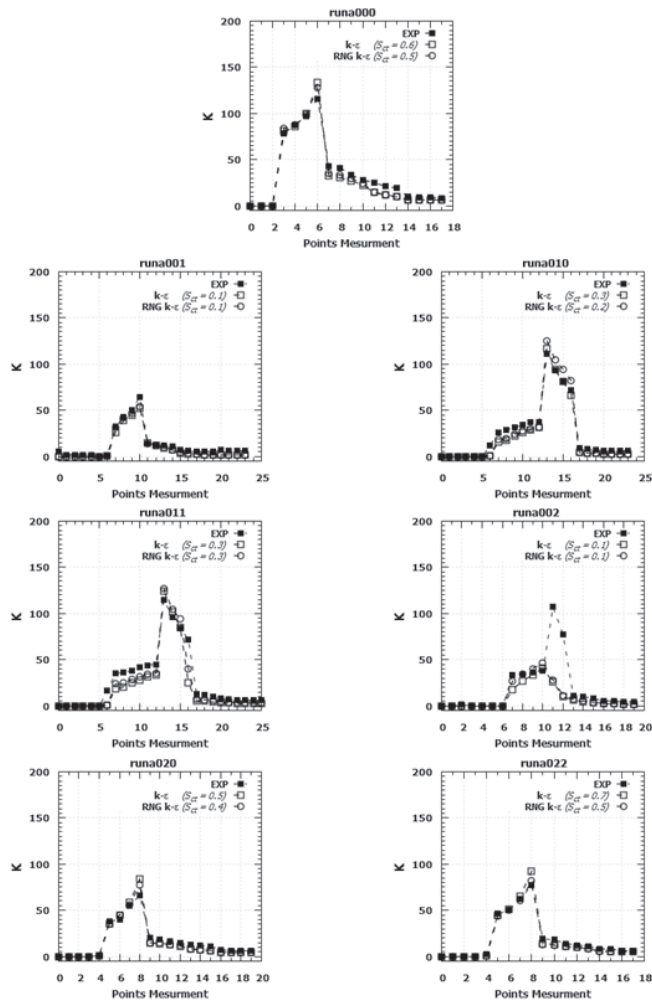


FIGURE 8. Dimensionless concentration  $K$ -distributions for all cases calculated with appropriate

ing good agreement with the wind tunnel results varies considerably from case to case. From the analysis of Figure 8 it can also be seen that for both turbulence models and secondly for the difference configurations, different appropriate turbulent Schmidt number leads to a good agreement between numerical results and experimental data, both for leeward and windward sides except for case runa002 where pollutant concentration is underestimated near the leeward.

The runa000 case is the most common configuration used to test and validate the CFD models used to predict the dispersion of pollution within street canyons. The geometrical configuration of the runa000 represents an idealized urban street canyon with an aspect ratio equal to one. There is many previous studies which investigate the mean flow characteristics and pollution field inside this simple configuration of street canyons.

As shown for runa000 case (Fig. 8 and Table 2), it appears that the  $Sc_t$  using RANS  $k-\varepsilon$  turbulence closure model represents the optimal value. This value is close to those used in the previous CFD research studies based on RANS  $k-\varepsilon$  turbulence closure model for the same case (Table 1). Theirs results also showed a better agreement with the experiment for  $Sc_t$  between 0.3 and 0.9. This slightly difference between  $Sc_t$  values for this same configuration may be due to different numerical approaches used by the researchers.

However, it should be noted that in previous numerical investigations (Table 1) this same constant value for turbulent Schmidt number is then adopted and used to evaluate pollutant dispersion in urban street canyons with various nu-

merical models and for different geometry configurations. The results obtained from this investigation have shown that there is an appropriate  $Sc_t$  for each case according to the geometry configuration of the street canyons and depending on the turbulence model used.

## Conclusions

After this analysis on pollutant dispersion, it is worth commenting that the large number of simulations, we performed for a wide range of turbulent Schmidt number values show evidence of a strong sensitivity on this relevant factor  $Sc_t$ , which makes a balance between two types of mass transport. We suggest to associate to each specific application on street canyon configurations its most suitable  $Sc_t$  values. This combination should certainly leads to the most approximated solution of the 2D configuration. In addition, the model of turbulence adopted for the simulations seems to have an impact on the choice of the appropriate  $Sc_t$ . The numerical results are compared with those of the experimental tests, a good agreement is observed. We proposed a summarized table giving values of  $Sc_t$  and models of turbulence which have to be combined with the corresponding 2D-idealised street canyons.

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## Summary

**A numerical analysis of pollutant dispersion in street canyon: influence of the turbulent Schmidt number.** Realizing the

growing importance and availability of motor vehicles, we observe that the main source of pollution in the street canyons comes from the dispersion of automobile engine exhaust gas. It represents a substantial effect on the micro-climate conditions in urban areas. Seven idealized-2D building configurations are investigated by numerical simulations. The turbulent Schmidt number is introduced in the pollutant transport equation in order to take into account the proportion between the rate of momentum turbulent transport and the mass turbulent transport by diffusion. In the present paper, we attempt to approach the experimental test results by adjusting the values of turbulent Schmidt number to its corresponding application. It was with interest that we established this link for achieving our objectives, since the numerical results agree well with the experimental ones. The CFD code ANSYS CFX, the  $k-\varepsilon$  and the *RNG*  $k-\varepsilon$  models of turbulence have been adopted for the resolutions.

From the simulation results, the turbulent Schmidt number is a range of 0.1–1.3 that has some effect on the prediction of pollutant dispersion in the street canyons. In the case of a flat roof canyon configuration (case: runa000), appropriate turbulent Schmidt number of 0.6 is estimated using the  $k-\varepsilon$  model and of 0.5 using the *RNG*  $k-\varepsilon$  model.

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