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# A Numerical Analysis on the Effect of Turbulent Schmidt Number on Numerical Prediction of Pollutant Dispersion within Street Canyons

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**Abstract**: This paper presents a numerical analysis on the effect of turbulent Schmidt number on numerical prediction of pollutant dispersion within street canyons. Four cases of idealised-2D street canyons were simulated with several modifications to buildings geometry. The $k-\varepsilon$ and *RNG* $k-\varepsilon$ turbulence closure models have been adopted for turbulence modeling and the accuracy of numerical predictions has been examined by comparing calculated results with the available wind-tunnel measurements. The simulation results showed that the turbulent Schmidt number is a range of *0.1* to *1.3* that has some effect on the prediction of pollutant dispersion in the street canyons. For each street canyon configuration, an optimum value for turbulent Schmidt number was determined which gives good agreement with the experimental results. In the case of a flat roof canyon configuration (case-00), appropriate turbulent Schmidt number of *0.6* is estimated using the $k-\varepsilon$ model and of *0.5* using the *RNG* $k-\varepsilon$ .

**Keywords:** Turbulence schmidt number, CFD simulation, Pollutant dispersion, Street canyons

## Introduction

Road transport emissions are a major of local source of air pollution in urban area. Thus far, modeling the outdoor urban environment and validation with experimental flows is a significant challenge for scientists and researchers. Several approaches have been developed and used over the past decades to study the flow field, pollutant dispersion and deposition inside urban street canyons. These methods include physical modeling, CFD and full-scale measurements of the wind flow and pollutants 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 et al. (2003), Ahmad et al. (2005), LI et al. (2006) and recently Tominaga et al. (2013) presents an overview of CFD procedures used to study wind and pollutants transport in the urban environment.

Physical modeling are conducted in order to study detailed information of the flow field and pollutants diffusion at reduced scales using different wind tunnels (Rafailidis et al. (1995), Meroney et al. (1996, 1999), Pavageau et al. (1999), Kastner-Klein et al. (1999), Baker et al. (2001), Kovar et al. (2002), Gromke et al. (2007)), water channel (Baik et al. (2000), Caton et al. (2003), Kim et al. 2005, Li et al. (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.

Due to increasing in computer performance, several 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 parameters such as street geometries, building roof shapes, thermal effects and trees planting (Sini et al., 1996; Rafailidis 1997; Theodoridis and



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Moussiopoulos, 2000; Xiaomin et al., 2005; Nazridoust and Ahmadi, 2006; Xie et al., 2005; Huang et al., 2009; Yassin, 2011; Salim et al., 2011; Gallagher et al., 2012; Tong and Leung, 2012; Takano and Moonen, 2013; Moonen et al., 2013; Liu and Wong, 2014; Ng and Chau, 2014; Madalozzo et al., 2014; Cui et al., 2014, Allergini et al., 2014, Efthimiou et al., 2015). Some of these CFD studies have been performed to investigate in detail the effects of building configurations on flows and pollutant dispersion. These studies often employ simple building configurations to study how the geometry and different roof shapes can affect airflow and pollutant fields in a 2D idealised street canyons (Theodoridis and Moussiopoulos, 2000; Chan et al., 2002; Assimakopoulos et al., 2003; Xiaomin et al., 2005; Nazridoust and Ahmadi, 2006; Huang et al., 2007; Huang et al., 2009; Yassin, 2011; Takano and Moonen, 2013). The most commonly RANS turbulent models used in street canyon simulations are the standard k – ε model, renormalization group RNG k – ε model and realisabled k – ε model and their performance are tested in some studies cited above.

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, and 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 (Thomas K. Flesch et al. (2002)). The turbulent Schmidt number $Sc_t$ is a fitting parameter that depends on the mean flow, turbulence fields and the spatial patterns of pollutant in street canyons (Koeltzsch, 2000, Blocken et al., 2008; Tominaga and Stathopoulos, 2013). Moreover, great importance in Air Quality Modeling within urban street canyons is the specification of a suitable turbulent Schmidt.

Our purpose throughout this study is to establish the link between a specific 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 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.

## Methods

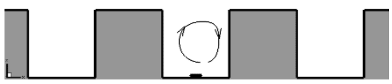
Computational investigations are performed using the CFD-code ANSYS CFX (ANSYS Academic Research, Release 16.2). In all simulations, the flow field is calculated using Reynolds Averaged Navier-Stokes (RANS) with the standard $k-\varepsilon$ (Launder and Spalding, 1974) and $RNG\ k-\varepsilon$ (Yakhot et al., 1992) turbulence models. For modeling the pollutant dispersion, an 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*.

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

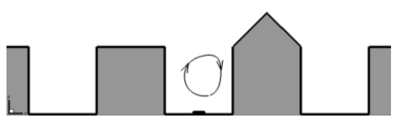
($C$ denote the pollutant mean concentration, $Sc_t$ and $\mu_t$ are the turbulence Schmidt number and the turbulence viscosity, respectively. $D_C$ is the molecular diffusivity coefficient of the pollutant).

### Computational Domain and Grid Generation

In order to analyse the influence of the turbulent Schmidt number on numerical predictions of pollutants dispersion in street canyons, four geometrical configurations are defined as indicated in fig. 1.



case-00



case-01


Figure 1. Street canyon configuration cases

All cases (Fig. 1) considered in this investigation have been studied experimentally by Rafailidis and Schatzmann (1995), and 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.unihamburg.de/fileadmin/files/static_html/ windtunnel/.

In the present study, five street canyons are considered in the computational domain (Fig.2). 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 domain dimensions are $11H \times 10H$ 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 that the CFD model is independent of the mesh size before a final mesh is selected. The total number of generated cells is about $25000-40000$ elements with $30 \times 30$ cells are placed in each street canyon as recommended by Ref. (Franke et al., 2007).

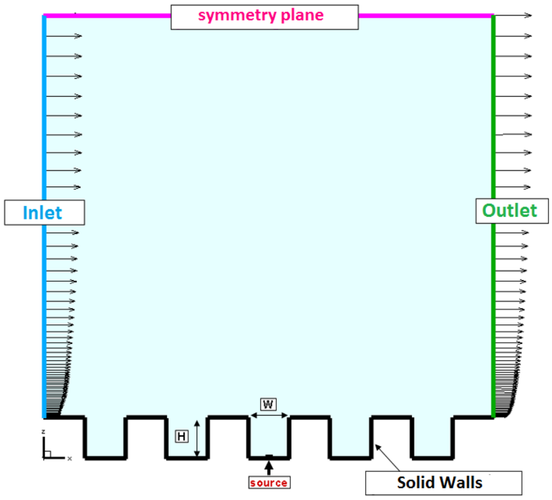
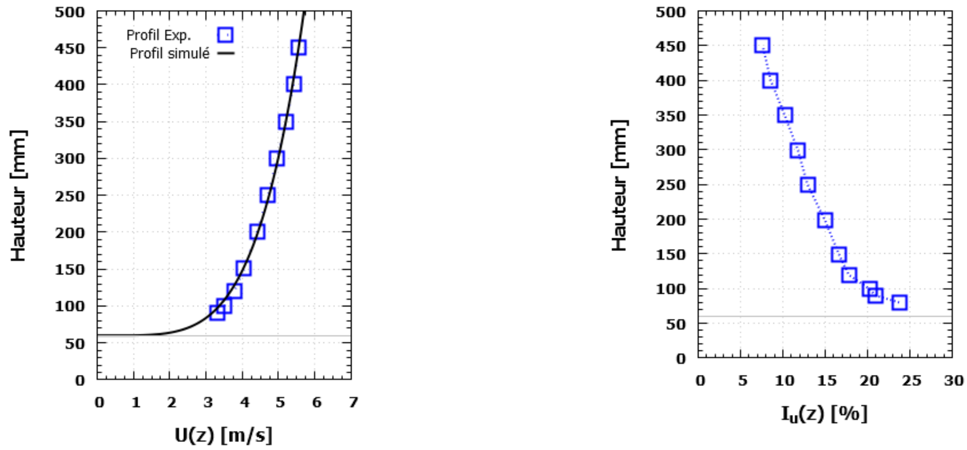



Figure 2. Computational domain

In the streets, the minimum cell size is of $1mm \times 1mm$ (applied on the building surfaces and the grounds) increasing gradually to a maximum of $2.5mm \times 2.5mm$ (in the middle of the 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 analysis, identical boundary conditions for airflow and pollutant are adopted (Fig. 3). At the inflow boundary, the measured distributions of longitudinal wind velocity $U(z)$ and the turbulent intensity $I(\%)$ are used.




velocity inlet profile $U(z)\ [m/s]$ Turbulent intensity inlet profile $I_u(z)[\%]$

Figure 3. Inlet boundary conditions

The turbulence kinetic energy and dissipation are estimated as $k_{inlet} = \frac{3}{2} I_z^2(z) U^2(z)$ and $\varepsilon_{inlet} = k_{inlet}^{3/2} / l_t$, 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 experiments conducted at the Meteorological Institute of Hamburg University (Rafailidis, 1995).

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. The pollutant considered is in the form of a mixture of ethane $\left(Q_{C_2H_6} = 4\,l/h\right)$ and air $\left(Q_{Air} = 100\,l/h\right)$. 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 analyse, the numerical simulations are done for four 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*.
In this section, the CFD results of the mean velocity, and pollutant dispersion in street canyon with source are presented. These computed results for each geometry configuration of street canyon are compared with experimental measurements of Rafailidis and Schatzmann (1995), and the influence of the turbulent Schmidt number on pollutant passive scalar predictions is discussed.

### Flow Field in Street Canyons

In fig. 4, we present the streamlines of mean velocity fields obtained from the numerical simulations of all cases (case-00 to case-11). 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.

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 center differ for each case. These differences produce different velocity contours and consequently a significant influence on pollutant distribution in street canyon. Predicted velocity fields have shown that the two turbulence models, $k-\varepsilon$ and *RNG* $k-\varepsilon$, give very similar air velocity fields. For the case-00 configuration only one main vortex, rotating clockwise, is formed at the center of the street canyon.

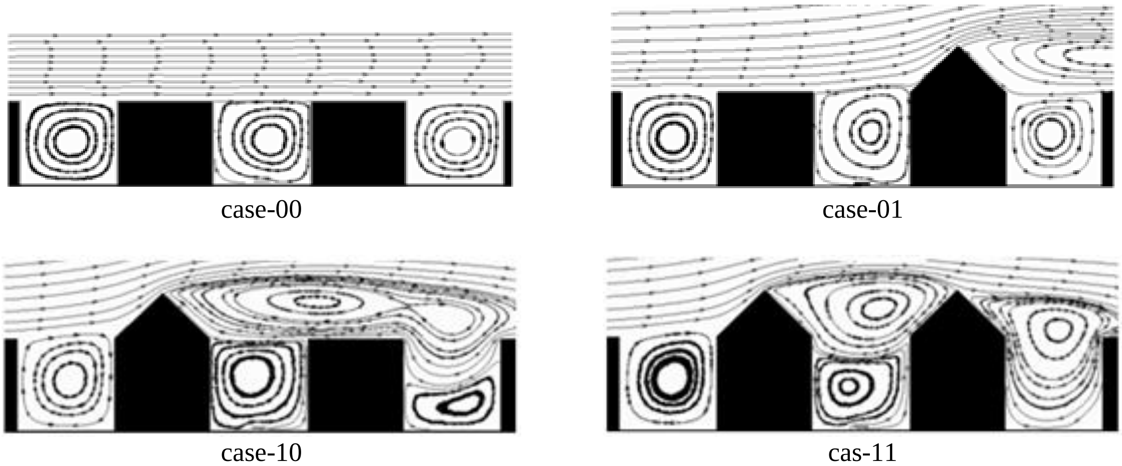



Figure 4. Streamlines in street canyon (obtained with the standard $k - \varepsilon$ model)

A similar vortex structure is found in case case-01 configuration of street canyon, but the main vortex is distorted and shifted towards the downstream building side. In the cases case-10 and case-11, 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.

**Analysis of Dimensionless Pollutant Concentrations**

In fig. 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 can be seen that *RNG* $k - \varepsilon$ model gives higher concentration than the $k - \varepsilon$ 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 turbulence model. As $Sc_t$ increases, calculated dimensionless pollutant concentrations $K$ increases on both side of the street with source for both $k - \varepsilon$ and *RNG* $k - \varepsilon$ turbulence models in all cases.

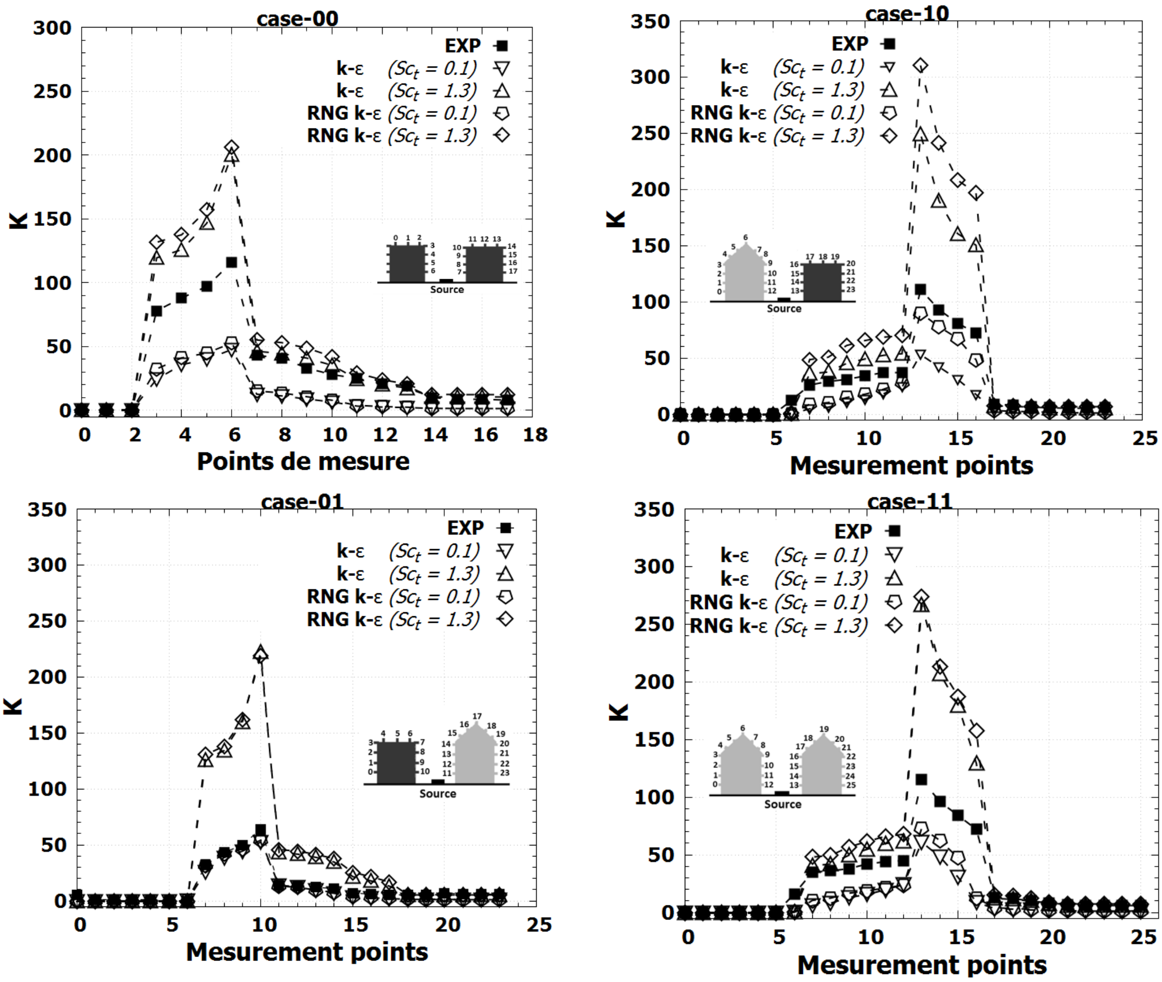



Figure 5. Dimensionless concentration *K* distributions for all cases

**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. The SER 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:

$$SRE = \frac{\sum_1^n \left| K_{i,Exp} - K_{i,Sim} \right|}{\sum_1^n K_{i,Exp}} \tag{2}$$

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

In fig. 6, we show a comparison of the relative error calculated for reference configuration (case-00). It can be seen that the appropriate turbulent Schmidt number corresponding to the minimum error obtained using $k-\varepsilon$ model is 0.6 and it is 0.5 when using $RNG\ k-\varepsilon$ turbulence model.

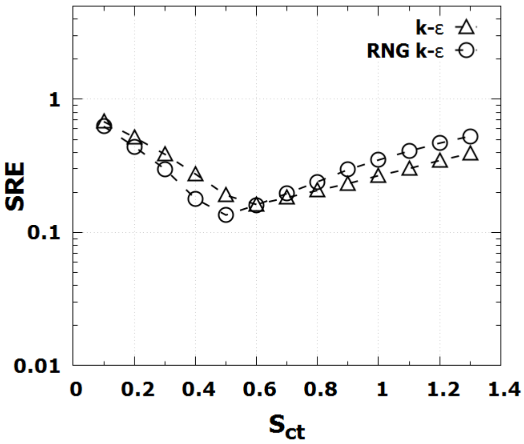
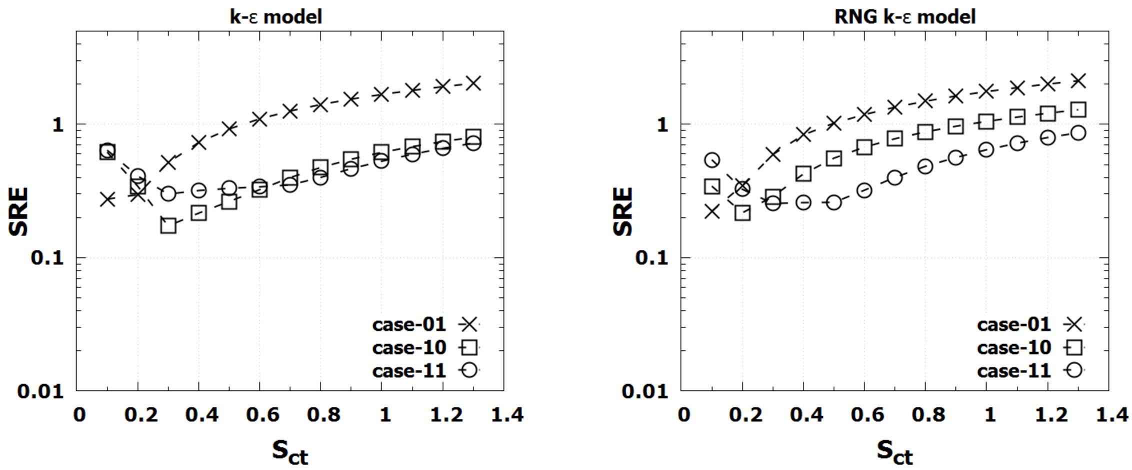



Figure 6. Sum of the relative errors for case-00 calculated for both $k - \varepsilon$ and *RNG* $k - \varepsilon$ turbulent models

The results presented in fig. 7 show that the appropriate $Sc_t$ number is strongly dependent on the turbulence model and on the street canyon geometrical configuration. We can notice a significant differences in appropriate Schmidt number value when changing the configuration of the street canyon.




(a) (b)

Figure 7. Sum of the relative errors for cases: Case-01, case-10, case-11 (a) calculated for $k - \varepsilon$ turbulent model, (b) calculated for *RNG* $k - \varepsilon$ turbulent model

It can also be observed that the appropriate Schmidt values corresponding to the model $k - \varepsilon$ and the model *RNG* $k - \varepsilon$ are almost identical. For all cases, appropriate $Sc_t$ values varied between 0.1 and 0.6 for $k - \varepsilon$ model and between 0.1 and 0.5 for *RNG* $k - \varepsilon$ model.

Fig. 8 presents a comparison of the experimental and simulation results for all cases, using both $k - \varepsilon$ and *RNG* $k - \varepsilon$ turbulence models. The profiles 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 providing good agreement with the wind tunnel results varies considerably from case to case. From the analysis of Fig. 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.

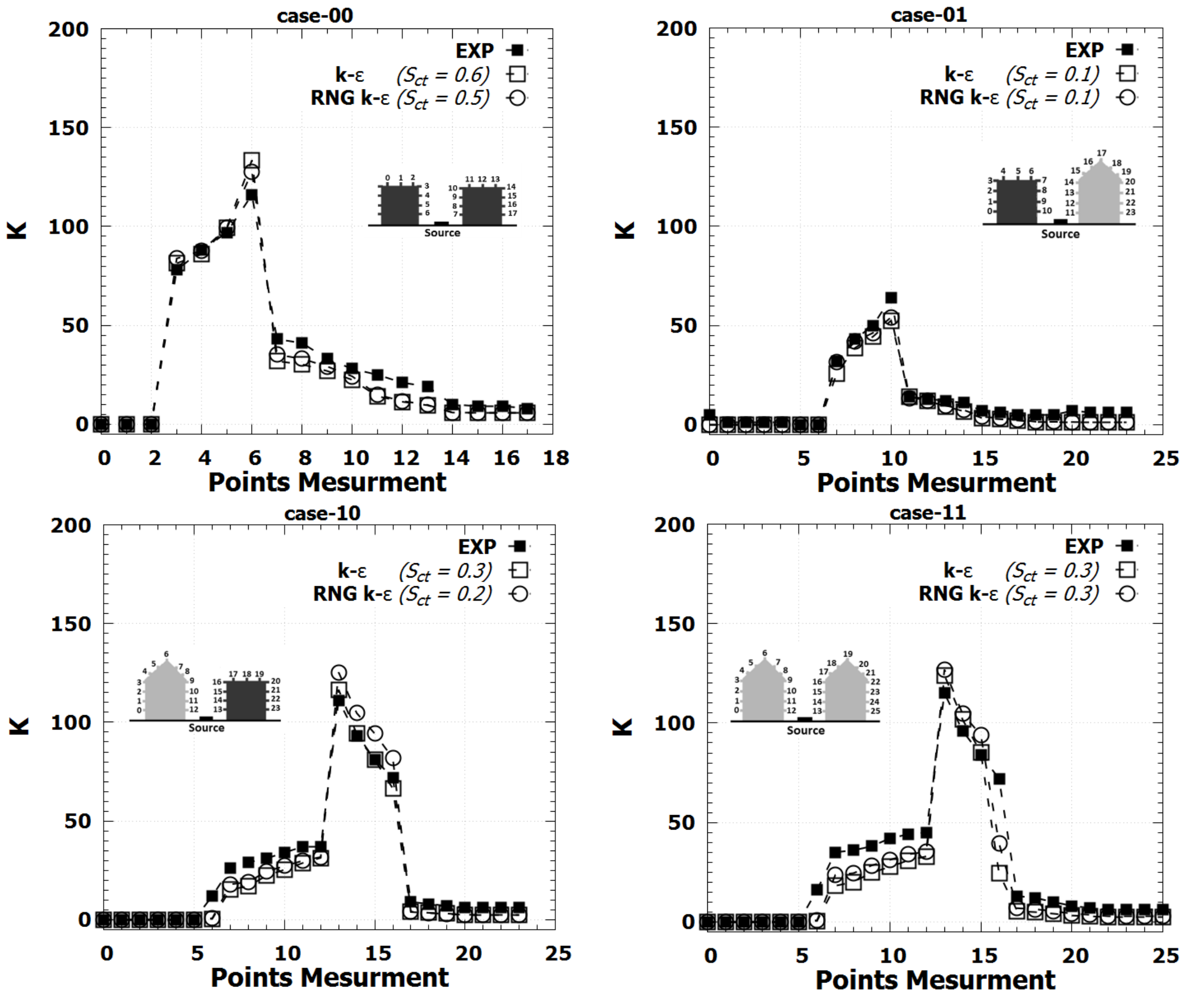



Figure 8. Dimensionless concentration *K* distributions for all cases calculated with appropriate $Sc_t$ .

The case-00 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 case-00 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 idealised-2D configuration of street canyons.

As shown for case-00 (Fig. 8), 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. 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 (Sini et al. (1996), Baik et al. (2000), Huang et al. (2000), Yassin et al. (2011), Baik et al. (2002), Gromke et al. 2008, Huang et al. (2009), Takano et al. (2013), Huang et al. (2015), C. Gromke et al. 20015).

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 numerical 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 numerical analysis on pollutant dispersion in idealized-2D street canyons, 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 lead 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 giving values of $Sc_t$ and two models of turbulence that have to be combined with the corresponding 2D-idealised street canyons.

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