RANS Passive Scalar Transport Modelling in a Complex Urban Area –
Effect of Source Location on the Results

Rakai, Aniko*¹), Berbekar, Eva¹), Franke, Jörg²,³)

¹) Department of Fluid Mechanics, Budapest University of Technology and Economics, Budapest, Hungary
²) Vietnamese-German University (V GU), Binh Duong New City, Vietnam
³) Department of Fluid- and Thermodynamics, University of Siegen, Siegen, Germany
*) presenting author, rakai@ara.bme.hu

ABSTRACT
The paper shows results of wind tunnel and RANS passive scalar transport modelling in a complex urban area, Michelstadt for three different source locations, one in an open square, one in a street canyon and one in a street intersection. Both continuous and short-term release results are compared. For the continuous release a turbulent Schmidt number dependency is investigated, while the short term results are compared to the measurement for two different mesh densities to show the dependency of the results on the spatial resolution. Results show that for different source locations no optimal turbulent Schmidt number value can be chosen even if the flow-field is the same, and the short-term release results are very sensitive to the mesh resolution.

1 INTRODUCTION
Passive scalar transport modelling with Computational Fluid Dynamics in urban areas is an important topic in Computational Wind Engineering as it can give detailed results on the dispersion of air pollutants or accidental releases, taking into consideration the effect of the complex flow field in an urban environment. On the other hand it still needs thorough investigation to increase its reliability and acceptance for regulatory purpose modelling. In this study the effect of source location on the results is investigated in a complex urban geometry, Michelstadt, which is an idealized Central European city centre, for continuous and short time releases.

2 TEST CASE
2.1 Wind-tunnel experiment
The Michelstadt test case, (Figure 1) is investigated in the framework of the COST Action ES 1006, Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments. Michelstadt is a 1:225 model of an idealized Central-European urban environment, with an approach flow characteristic for a very rough boundary layer, according to the roughness classification of the VDI (2000) guideline for wind-tunnel measurements. Tracer-gas releases from three ground-level sources were investigated in the Environmental Wind Tunnel Laboratory of the University of Hamburg. Results of continuous release concentration measurements are available in horizontal planes for all three sources and in three vertical profiles for source S2 (Figure 1). Furthermore, the dispersion of short-term (puff) releases from the same source locations were also measured (see red circles in Figure 2). The duration of the continuous release measurements and the number of the released puffs ensure the statistical representativeness of the results.
During the evaluation of the experiments, the measured concentration time series were converted to dimensionless and full scale values. To characterise them, different parameters were determined based on the time series. In this paper, the mean concentrations of the continuous release measurements are compared with the numerical results. For the puff release case, the dosage (the total amount of concentration at the measurement point during the measurement) and the peak time (the time between the beginning of the puff release and when the maximum concentration occurs at the measurement point) were defined for each puff released during the experiments (Harms et al 2011). Finally, both the dosage and the peak time were averaged for each measurement location, and the resulting mean dosage and mean peak concentration were compared with the numerical results. Furthermore, the time series of all puffs measured at the same location were averaged, and the concentration time series of the resulting so-called mean puff is also used in this paper as a basis of a qualitative comparison. More details about the experimental setup and the measurement results can be found in Berbekar et al (2013).

![Figure 1: Top view of the investigated test case, Michelstadt, with 3 source locations S2, S4 and S5, and the corresponding concentration measurement locations.](image1)

![Figure 2: Closer look on the source and measurement locations, with a red circle around the measurement points where finite duration emissions, i.e. puffs, were also measured.](image2)
2.2 Numerical setup

Dispersion calculations were carried out in a constant flow field previously calculated with Reynolds Averaged Navier Stokes (RANS) modelling using OpenFOAM 1.7. More detail on the flow modelling can be found in Rakai et al. (2014).

A passive scalar pollutant was assumed and the turbulent scalar flux was modelled with the simple gradient diffusion hypothesis. The effect of turbulent Schmidt number \( (Sc_t) \) was investigated by carrying out calculations with its value varying from 0.1 to 1 with 0.1 intervals. More details on dispersion modelling can be found in Rakai and Kristof (2013), with a grid sensitivity analysis, but here only one body fitted hexahedral mesh generated by the snappyHexMesh utility of OpenFOAM with 2.4 million cells was used for \( Sc_t \) dependency analysis due to computer resource constraints.

Puffs were modelled also in the constant flow field, with a short-term release duration equal to the one in the measurement. The resulting puff can be considered a mean puff, and will be compared to the ensemble mean of the puff time series at each measurement location. For this exercise \( Sc_t=0.7 \) was used for all the source locations, and a very coarse polyhedral mesh with 1.73 million cells (coarse) and a very fine body fitted hexahedral mesh with 27.52 million cells (fine), to have a first impression on the grid sensitivity of puff modelling. A more precise description of the meshes can be found in Rakai et al (2014).

3 RESULTS AND DISCUSSION

3.1 Continuous emission

Continuous emission results are compared with a normalised concentration value, \( c^* \), defined in Equation (1), where \( c \) is the concentration, \( U_{\text{ref}} \) is the reference velocity used in the measurement and the simulation, \( L \) is reference height, and \( Q_{\text{source}} \) is the source strength.

\[
c^* = \frac{c \cdot U_{\text{ref}} \cdot L^2}{Q_{\text{source}}}
\]

For source S2, a source in an open square, results are compared in the left of Figure 3 at a height of \( z=7.5 \)m. Simulation results are shown as contour plot with the measurement results as discrete points for \( Sc_t=0.7 \). We describe the dependency of the results on \( Sc_t \) with the help of two simple metrics, \( L^2 \) and \( FAC2 \) (Equation (2) and (3) with \( E_i \) as experimental and \( S_i \) as simulation data in the \( N \)th measurement point of all the \( n \) measured points for each source), on the right hand side of Figure 3 as a function of \( Sc_t \). For easier comparison 1-FAC2 values are plotted, so the lower value means better for both metrics in the plot.

\[
L^2 = \frac{\sum_{i=1}^{n} (E_i - S_i)^2}{\sum_{i=1}^{n} E_i^2}
\]

\[
FAC2 = \frac{N}{n} = \frac{1}{n} \sum_{i=1}^{n} N_i \quad \text{with} \quad N_i = \begin{cases} 
1 & \text{for } 0.5 \leq \frac{S_i}{E_i} \leq 2.0 \\
1 & \text{for } E_i \leq W \text{ and } S_i \leq W \\
0 & \text{for else}
\end{cases}
\]
From Figure 3 it can be seen that the shape of the plume is similar in the measurement and the simulation, but the high concentration zone is more convected to the streamwise direction in the simulations, and it is not diffused enough in the lateral direction, see e.g. the first street canyon with a slight angle on the right. It could be argued that a lower Sc will help the lateral diffusion of the plume and thus give better agreement, but it can be seen on the left hand side of Figure 3 that both metrics result in an optimal value of $\text{Sc}_t=0.7$ for this source location, which is the one shown in the Figure.

![Figure 3: Contour plot of the normalized passive scalar concentration from simulations together with the experimental results as discrete points at measurement height $z=7.5\text{m}$ in full scale, for source 2, vectors of the flow field are also shown for experiment (black) and simulation (red)](image)

We followed the same procedure for source S4, a source in a street canyon. The results are shown in Figure 4, also for $\text{Sc}_t=0.7$ and the same height on the left hand side. Interestingly, here the opposite can be observed about the convected plume, the measured plume is convected more than the simulated. Note the pink squares in the orange region as opposed to the green squares in the orange region in Figure 3. For the lateral dispersion it can be seen that in the right direction the plume is not spread enough, while for the left, it is more spread for the simulations. This cannot be corrected by the $\text{Sc}_t$ number changes, but can be due to the error in the underlying flow field. For this source we have flow field measurements quite close to its location, the resulting vectors are also plotted in Figure 4. It can be seen that in the region of the first lateral street canyon after the source, the mean velocity vectors of the measurements and the simulation already differ, which can cause the difference in the convected plume. For the optimal $\text{Sc}_t$ for this source location, not only we can observe that 0.7 is not the best value anymore, but also we find a contradiction in the behaviour of the metrics. The results were double checked as it looks like a plotting error. No best choice can be given for $\text{Sc}_t$ in this case, and the metrics are in general higher, showing that this source location is more difficult to model.
The last investigated source location is source S5, in a street intersection, its results are shown in Figure 5. The size of the convected plume seems to be better predicted here by the simulation, but the lateral spread is problematic, just as in the case of S4. This behaviour can be expected as this source is exactly in the lateral street canyon where already the flow field modelling is difficult. For the optimal $Sc$ value in this case, 0.5, can be chosen by both metrics, but it can also be observed here that metrics are higher than for S2, showing that the source location is also more difficult than the open square, as could be expected.

Seeing the results of both 3 sources, it can be argued that even in the same geometry and flow field no general $Sc$ can be suggested, which calls for a method to define it as a local function of the flow-field, or to use a more elaborate model for the turbulent scalar flux than the simple gradient diffusion hypothesis.

For sources that are in difficult locations, like street canyons or street intersections, already the modelling of the underlying flow-field is difficult for a steady state RANS model, however that is an often used approach due to the large computational resource needed for the time dependent
modelling. In this case we have to be aware that the dispersion modelling results can be misleading due to the errors in the flow-field.

3.2 Short term release

We move to an even more demanding exercise for the RANS model, as in case of the short term release puff modelling results are compared not only in space, but also in time. First a qualitative comparison is shown in Figure 7, where the calculated mean puffs are compared at each receptor location. As the puff modelling is not as demanding as the $Sc$ number optimization, for this investigation a simple grid sensitivity is shown with a very coarse and a very fine mesh. In Figure 7 we can observe that for source S2, which is an easier source in an open square, the results of the two meshes are similar. However for the other two, difficult sources, the results of the finer mesh are clearly better. In case of the very coarse mesh, the calculated plume has probably a different direction, missing both receptor points in case of S4, and receptor point P9 in case of S5.

![Figure 7: Comparison of a mean puff from measurements (WT – black plus sign) and from the RANS simulation with coarse polyhedral (red solid line) and fine hexahedral (blue solid line) grid.](image)

To give a more quantitative comparison, mean dosage and peak time values are compared in Figure 8 for all receptor locations. It can be observed that for source S2 the results are even slightly better for the coarse mesh. The puffs at receptor point P7, which is in the streamwise street canyon, and P22, which is in the second right hand lateral street, are overpredicted, while at P19, in the first right hand side lateral street, there is an underprediction, probably because the flow does not turn enough into that direction in the simulations. The higher numerical diffusion of the coarse mesh can help to diffuse the plume more to that direction, thus improving results in a misleading way, giving a right answer for the wrong reason. For S4 and S5 the results of the finer mesh are clearly superior.

To give an even deeper insight into the puff modelling and its difficulties, histograms of the distributions of the measured results for approximately 200 puff measurements per receptor point are shown in Figure 9 together with the mean value of the measurements and the simulation values for one receptor point per each source. It can be seen that the distribution for the dosage is right-skewed, therefore the mean value does not correspond to the most probable value with the
highest bar in the histogram. It is a difficult question to decide whether the results of the simulation should be compared to any other statistical value of the distribution, but we decided to compare the mean values, as the result of a RANS simulations is a Reynolds averaged value, so comparing to other than the average would add additional uncertainty to the comparison.

Figure 8: Comparison of two puff parameters, mean dosage and peak time (The mean peak time of the wind tunnel results at P10 of S5 is missing due to measurement problems.)

For the peak time distribution this question is not so difficult, as their distribution is less skewed. An interesting thing to note is that in case of the receptor point P5, the coarse mesh gives a value which is an outlier but was present in one of the puff measurements. As the flow-field in the wind tunnel is turbulent, the 200 puffs measured to give this distribution had different plume directions, and one of them could be similar to the one modelled by the coarse mesh. This does not justify the use of coarse meshes, but reminds to the large variability of the short term release modelling, and that it is a very difficult task to model properly, also in the wind tunnel.

Figure 9: Histogram of the puff statistics for dosage and peak time values, showing the computed mean value and the calculated values from the computations, for one receptor point for each source
4 CONCLUSIONS

Passive scalar transport modelling with the RANS approach in a complex urban geometry, Michelstadt, was investigated with the help of comparing continuous and short term releases to wind tunnel measurements. Three different source locations were compared, one in an open square, one in a streamwise street canyon and one in a street intersection to see the effect of the location in the results. Based on two different statistical metrics, it can be said that the easiest source to model is in the open square.

The effect of changing turbulent Schmidt number in a systematic way was also investigated. For source S2 the default value of the turbulent Schmidt number, 0.7, gave the best results based on statistical validation metrics, however for the other two sources different optimal values were found. So even in exactly the same geometry and flow field different source locations may require different turbulent Schmidt numbers, calling for a flow field dependent value or more complex dispersion modelling.

The short term release modelling with the steady approach was also investigated with a preliminary grid sensitivity analysis. It was found that this approach has a strong dependency on both the location of the source and the grid resolution, and still leaves a lot of open questions for this kind of modelling. For the relatively easy-to-model source in the open square the coarse mesh gave better results for the two investigated statistical puff parameters, the dosage and the peak time, giving a better answer for the wrong reason, possibly numerical diffusion. For the other two source locations the fine mesh had outstandingly better results for the compared mean statistical parameters.

Short term release modelling is an important question in emergency response modelling, it is in the focus of COST Action ES 1006, Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments. To have more confidence in the steady state RANS approach in puff modelling, a more elaborate grid sensitivity study with a way to quantify numerical uncertainty in the simulation results, together with the experimental uncertainty, and a more thorough investigation of the statistical distribution of the puff parameters would be necessary.

Acknowledgements
The measurement results from the COST ES 1006 action are gratefully acknowledged. The research was financed by the K 108936 ID project of the Hungarian Scientific Research Fund, by the Deutsche Bundesstiftung Umwelt and by Campus Hungary grants ID: 46851 and B1/1R/396.

References