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Applicability of Gaussian dispersion models for accidental releases in urban environment – results of the "Michelstadt" test case in COST Action ES1006

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Abstract. One of the main research tasks of COST Action ES1006 was testing available dispersion models in order to evaluate their applicability in real situations of accidental gas releases in urban environment. For that purpose, model inter-comparison as well as comparison against test data from wind-tunnel experiments was performed.

Because of the characteristics of the wind flow in urban conditions, such as recirculation and/or blowing through the street canyons, the influence of high buildings and the relatively higher overheating at the surface, the use of more complex models is necessary. When it comes to complexity however, some questions are to be considered:

- What computer resource does the chosen model demand? For emergency response, minimum time for processing the input data combined with maximum output resolution of the pollution field would be a decision for a part of the problem.
- Is the model adequate enough to handle, and to what degree could it represent, the situation of emergency: input/output issues – meteorology, number of sources and receptors, specifics of the pollutant etc.

When Gaussian models were applied for the "Michelstadt" experiment, namely AERMOD, TRACE and ALOHA for the sake of emergency response, a very simplified output was achieved at minimum input requirements. TRACE and ALOHA showed similar sensitivity to wind direction, due to the relatively narrow plume simulated by both models. The best concentration predictions for continuous releases were observed when the wind flow direction was rotated -5°

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(5° counter-clockwise in relation to 0° direction). The tests with varying surface roughness (0.5, 0.8, 1.0 and 1.25 m) gave negligible differences both with ALOHA and TRACE.
Being an integrated system, the AERMOD dispersion model is more complex. So, besides the sensitivity to surface roughness, the sensitivity of AERMOD to flow direction and friction velocity values was investigated. Changing the wind direction with -5° and -10° improved the prediction at the near source receptors. Reducing the friction velocity by 71% ($u_* = 0.4$ m/s) compared to the initial one ($u_{*0} = 0.566$ m/s) improved the concentration prediction at the near source receptors and at some distant receptors.

Keywords: air pollution, model evaluation, Gaussian models, accidental releases, wind-tunnel data, sensitivity test.

1. INTRODUCTION

With the process of industry development and urban area spreading, some corresponding changes in the factors that influence dispersion of air pollutants take place. An example for a typical city evolution scenario and its concomitant air pollution problems, is an industrial facility which in a distant time in the past had been situated out of the populated area, but with the city expansion it fell into it. The transition from a rural to an urban canopy with its newly constructed buildings, streets, fittings and installations, modifies the physical conditions which heavily affect the wind speed and especially the wind direction around these obstacles (Britter and Hanna, 2003; Oke, 1996; Venegas et al., 2014). As a result, conditions for downwashing and trapping of pollutants into the so called "street canyons" are created. Furthermore, the modified urban canopy yields micro-climate changes – not only in the examined domain, but in its neighboring areas as well.

Nowadays, an increasing interest in studies and discussions over scenarios involving accidental releases in urban environments takes place (COST ES1006, 2012). The source of such releases could be an industrial accident, fire, explosion or a toxic chemical spill. Buildings and other obstacles disturbing the wind flow are better described by CFD (computational fluid dynamics) and Lagrangian coupled with CFD models which consume larger computational power and time resources, and which are still not practical for use as emergency response tools. On the other hand, Gaussian dispersion models requirements are low, but at the expense of accuracy. In this paper, three Gaussian models – AERMOD, ALOHA and TRACE are examined for emergency response applicability by comparison between model output data and wind-tunnel data.

2. DESCRIPTION OF WIND TUNNEL EXPERIMENT

Within the scope of COST Action ES1006, the large boundary layer wind tunnel facility "WOTAN" at the Environmental Wind Tunnel Laboratory of Hamburg University was used for the experiments. A neutrally stratified model boundary layer flow was generated by a carefully optimized combination of turbulence generators (so-called "spires") at the inlet of the test section, and a compatible floor roughness.

The extended "Michelstadt" wind tunnel experiment (Fischer et al., 2010) was designed as the first application-specific test case for the validation of local scale emergency response models. The building structure named "Michelstadt" represents an idealized Central-European urban environment. Figure 1 indicates the urban layout that was developed and used for model evaluation. Flow and concentration measurements were carried out in selected relevant locations with a higher density of data close to the ground. Measurements were collected for seven release scenarios corresponding to different point source locations and two different wind directions. Both continuous and short-term (puff) releases were carried out. Flow and concentration data were made available in a first "open" test case for the modeling exercise. In a second "blind" test, only minimum information on inflow data and the emission description were provided to the modelers. For the sake of briefness and for clarity, only the "non-blind" test with continuous releases from one point source (with ID "S2") is described here.

Fig. 1. "Michelstadt" urban layout developed in the wind tunnel "WOTAN" and used for model evaluation.

3. MODEL RUNS

3.1. Used input data

The input used for ALOHA, TRACE and AERMOD models is given in Table 1. Sensitivity tests with changing of the wind direction (+ / – 5°) were made. The main difficulties with ALOHA and TRACE data assimilation were, that the receptor data could only be entered manually (no batch allowed), which was time consuming.

Table 1. Used input for ALOHA, TRACE and AERMOD

Source input – continuous release	
Type of pollutant	C_2H_6 (ethane)
Source locations (x, y, z)	Source "S2" at (0.0, 0.0) m for ALOHA and TRACE, and (-361.9, 125.1) m for AERMOD
Source diameter	1.575 m (TRACE, AERMOD)
Source volume flow rate	0.4 m^3s^{-1} (ALOHA, AERMOD)
Source mass flow rate	0.5 kgs^{-1} (TRACE, AERMOD)
Temperature of the source's exit gas, T	293.15K
Receptor input	
Discrete receptor locations	Taken from database and transformed to meet the source locations (ALOHA, TRACE) or left as they are (AERMOD)
Receptors flagpole height	7.5 m for TRACE and AERMOD and 0.0 m for ALOHA
Receptor grid origin	ALOHA and TRACE: Coincides with the source; AERMOD: (x,y) = (0.0, 0.0) m – the center of Michelstadt domain
Meteorological input	
Wind velocity at 9 m height	2,7 ms^{-1}
Wind direction at 9 m height	270.0° (sensitivity tests: -5°, +5° – counter-clockwise and clockwise rotation in relation to 270° direction accordingly)
Ambient temperature at 2 m height	293.15 K
Relative humidity	50 %
Surface roughness length	0.8 m (sensitivity tests in the 0.8 – 1.2 m interval show almost no change in output)
Pasquill stability class Inversion height options	D (Neutral)(ALOHA, TRACE) Set to "No inversion" (ALOHA, TRACE)
Monin-Obukhov similarity (AERMOD)	u_* = 0.35, **0.4**, 0.45, 0.5 and 0.566 ms^{-1}

TRACE always sets the $\boldsymbol{x}$ coordinate axis downwind the source, so in order to make wind change sensitivity tests in absolute coordinates, the rotation matrix (Eq. 1) had to be applied:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{1}$$

where $\theta = +/-5\,^{\circ}$ is the angle of rotation. As a result, any change of coordinates in that manner yields the need of additional receptor input for the TRACE model.

Neither ALOHA nor TRACE need vertical wind profiles for the meteorological input (Reynolds, 1992; Thoman et al, 2006). The wind speed value of 2.7 ms^{-1} (at 9 m reference height, in full scale) was taken from the vertical wind profile database, situated in Michelstadt domain at coordinates (–450, 112.5 – see “Profile 2” location on Figure 2). This point would be the most representative for the meteorological input, since it was within the domain, and the wind direction at that point was not directly influenced by any situated buildings in the vicinity. Another advantage was, that the point was close to the source “S2”, (coordinates –361.9, 125.1).

AERMOD requires vertical wind and temperature profile data in a separate file (e.g. “aermod.pfl”). The profile may be consisted of data which is limited to as little as one layer (e.g. the temperature and wind at 2 m height only), but the more detailed the data is (if available), the more accurate the output results would be. The sensitivity tests made were more extended: –10°, –5°, +5°, and +10° for the wind direction, 0.566ms^{-1} (100% u_{*0} – the approach flow friction velocity scale), 0.5 ms^{-1} (88% u_{*0}), 0.45 ms^{-1} (80% u_{*0}), 0.4 ms^{-1} (71% u_{*0}), and 0.35 ms^{-1} (62% u_{*0}) for the friction velocity scale, and 0.5, 0.8, 1.0, 1.25 and 1.5 m for the surface roughness z_0. Here, only the cases with u_{*0} = 0.4 ms^{-1} and z_0 = 0.8 m are shown, since they have the best match with the wind tunnel measured data.

3.2. Performance of the models

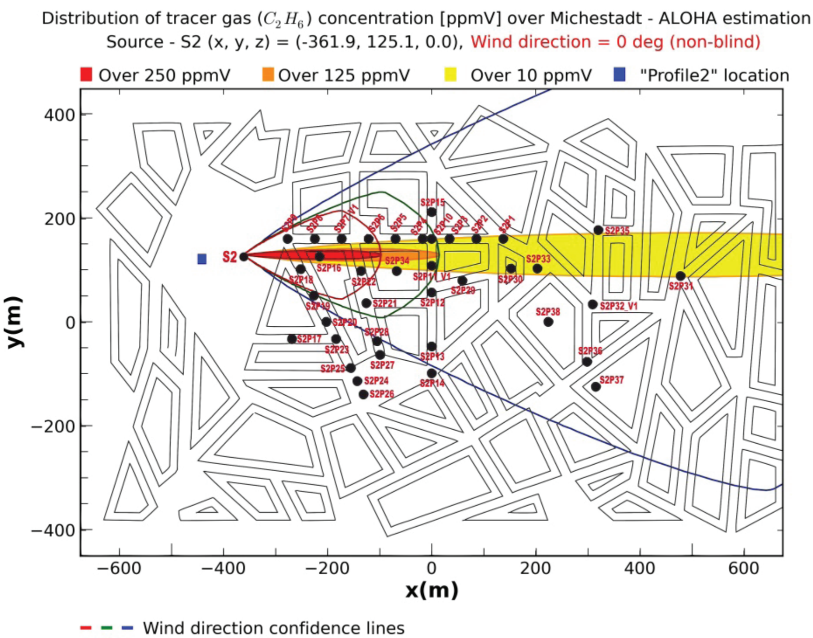
Developed for emergency response, both ALOHA and TRACE had almost instantaneous output for an arbitrary receptor when run under Windows 7 OS on a i3 dual core machine with 4GB RAM. The only impediment was when larger number of receptors were needed for examination. For TRACE, there is limitation to 20 receptors for a model run. One very good feature of the model is the option to perform sensitivity tests for various parameters (surface roughness, stability, etc.), except for wind direction variations. For ALOHA, coordinates for only one receptor can be given as an input for a model run. However, there is an option to see the concentration of the pollutant at any point interactively.

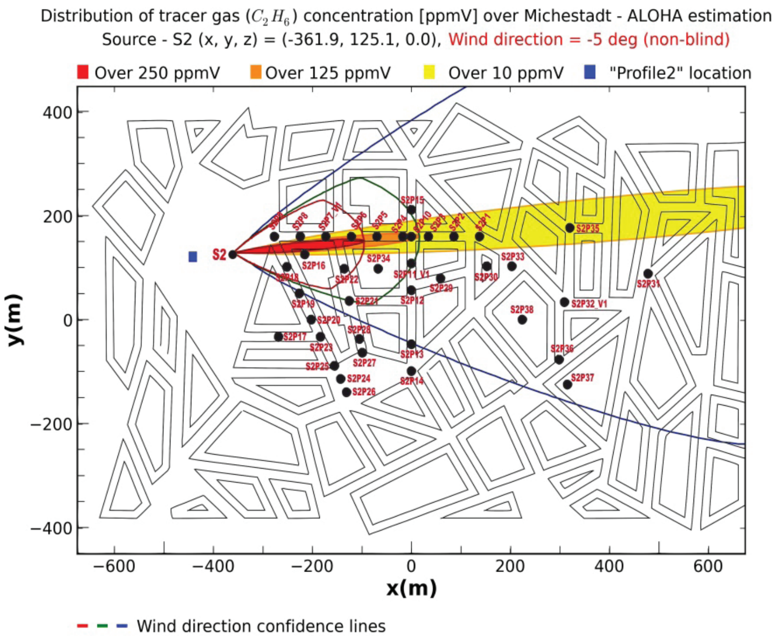
AERMOD has instantaneous output as well, with the difference that the model allows setting of receptor grid with an arbitrary resolution, and the number of discrete receptors to be defined could be practically unlimited. AERMOD is an open source model. It could run on any Windows or Linux machine. Since the model is intended for regulatory purposes it has some limitations in its use as an emergency response tool: it cannot handle short term ("puff") releases, as its minimal temporal resolution is 1 hour, and the input data files preparation is time consuming.

4. OUTPUT RESULTS, DATA COMPARISON AND STATISTICS

4.1. ALOHA

On Fig. 2 ALOHA's outputs for continuous releases are shown for three cases. Figure 2 (top) shows the "ordinary" (0°) non-blind scenario, Fig. 2 (middle and bottom) – the wind direction change sensitivity (–5° and +5°) test outputs. The contour lines colored in red, green and blue are the wind direction confidence lines. They show the possible mean concentration of the pollutant within the area enclosed by them in case, that wind direction fluctuations in the +/– 30° interval occur.





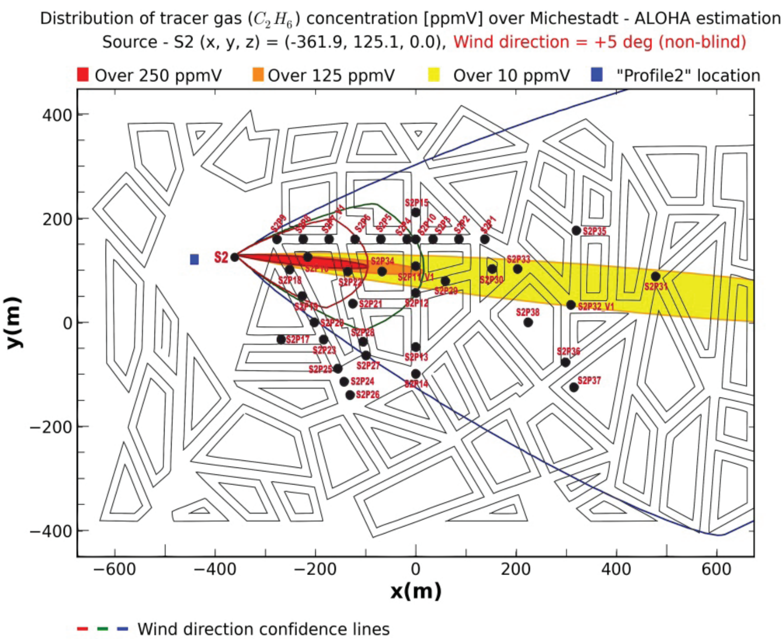


Fig. 2. Wind direction sensitivity of ALOHA; top is for 0°; middle for – 5°; and bottom for +5°

For the puff releases, the picture would be the same with the reservation that the displayed values of the concentration of the pollutant are relevant to the *peak* concentration.

The comparison between the images which show the distribution of the pollutant reveals very high sensitivity of the model to wind direction change. This becomes even more obvious if we take a look at the graphical expression of the comparison between the three specific cases on Fig. 3:

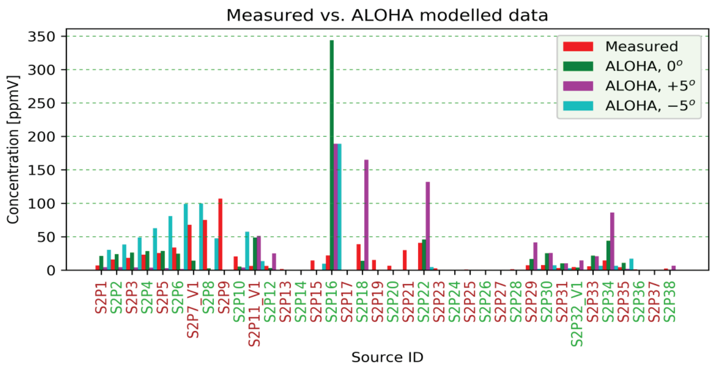


Fig. 3. Comparison between ALOHA's estimated (0°, +5° and –5°) and wind tunnel measured concentrations [ppmV] for source S2

Interesting situation occurs at point S2P16. It is located exactly downwind the source S2, at the centerline of the plume, and therefore the highest pollutant concentration is observed there. The +5° and the –5° wind direction sensitivity tests show identical results due to distribution symmetry. The estimate concentrations for the receptor point S2P9 which is the closest to the source S2, show values near to zero. If we look at Fig. 2, we could see that the width of the plume is very small, hence the receptor point S2P9 is very weakly affected by the source. The same goes for the points S2P2 to S2P10, in the case when the wind direction is slightly rotated clockwise (+5°), and for S2P18, S2P19, S2P21, and S2P22 in the counter-clockwise rotation (–5°) case. Only the results of S2 receptor set are discussed here, for the reason that it involves the largest number of receptors and covers the largest area of the Michelstadt domain.

One of the best ALOHA model's output features that come in handy, are the wind direction confidence lines. Even though not directly, they can show that the point S2P9 mentioned above could get into a zone with pollutant concentration exceeding 250 ppmV.

The statistical performance measures (SPM) used in the comparison were:

$$\mathrm{FB} = \bar{c}_0 - \bar{c}_p / 0.5(\bar{c}_0 + \bar{c}_p) \tag{2}$$

$$\text{NMSE} = \overline{(c_0 - c_p)^2} / \overline{c_0 c_p} \tag{3}$$

$$R = \overline{(c_0 - \bar{c}_0)(c_p - \bar{c}_p)} / \sigma_{c0}\sigma_{cp} \tag{4}$$

$$FAC2 : 0.5 \le c_0 / c_p \le 2.0 \tag{5}$$

where FB is the fractional bias, NMSE – the normalized mean square error, R – the correlation coefficient, FAC2 – the fraction of predictions within a factor of two of observations, c_o and c_p are the wind tunnel and modeled concentrations respectively, and σ_{co} and σ_{cp} – their corresponding standard deviations. The four SPM for ALOHA are shown in Table 2:

Table 2. ALOHA statistics for continuous releases

SPM	Wind direction	0°	–5°	+5°
NMSE		10.23	4.22	6.62
R		0.06	0.32	0.14
FB		-0.19	-0.27	-0.23
FAC2 (%)		21.05	15.79	2.63

According to statistics, the best match between measured and modeled data for the source S2 is observed in the case of wind direction shifted with -5° (counter-clockwise rotation).

4.2. TRACE

On Fig. 4. the graphical output for a continuous release provided by the TRACE model is shown, and on Fig. 4 - for the three cases involving wind direction sensitivity tests (plotted with Python 2.7.5 Matplotlib library; Tosi, 2009). TRACE supports pollution dispersion modeling for a horizontal plane, situated at any arbitrary height (ALOHA makes this only at ground level z = 0.0 m). For that reason, the statistical analysis for S2 includes the receptors situated on different flagpole heights (S2P7_V2 – S2P7_V7, S2P11_V2 – S2P11_V7, S2P32_V2 – S2P32_V5).

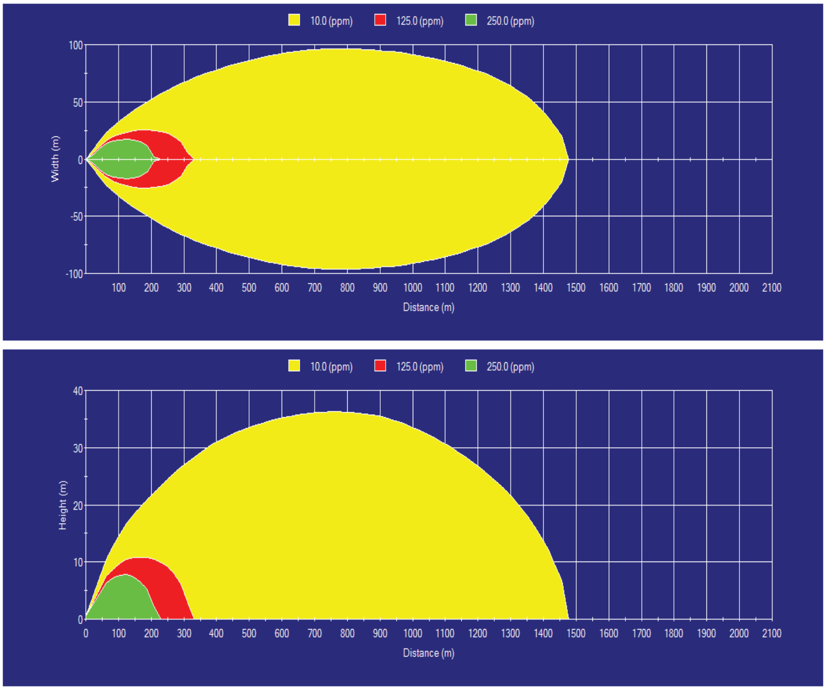
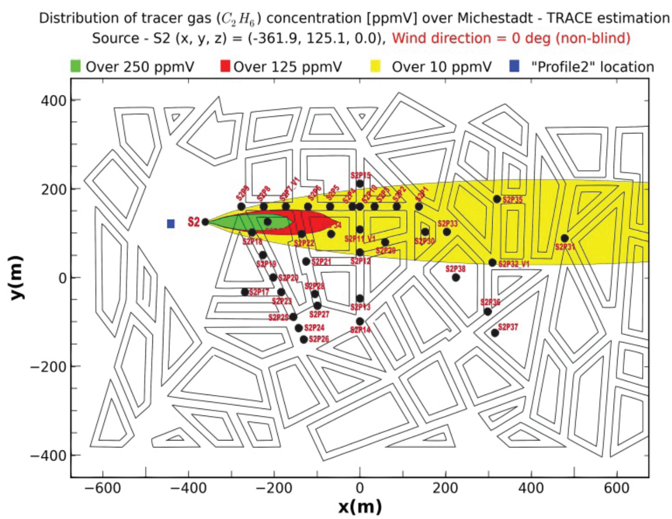
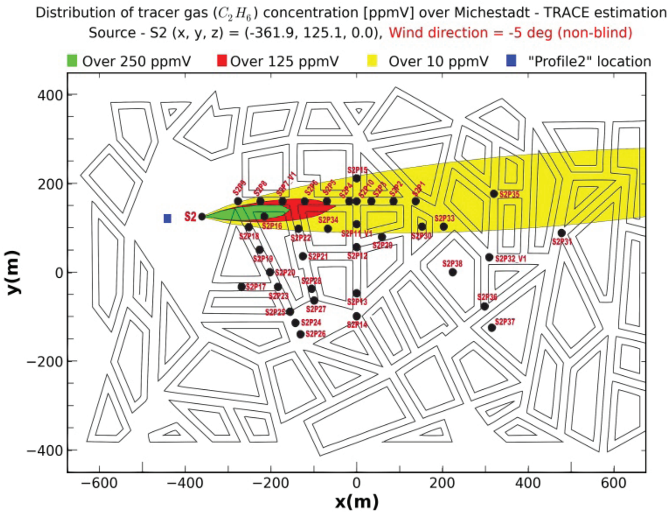


Fig. 4. TRACE direct graphical output (horizontal and vertical plane)





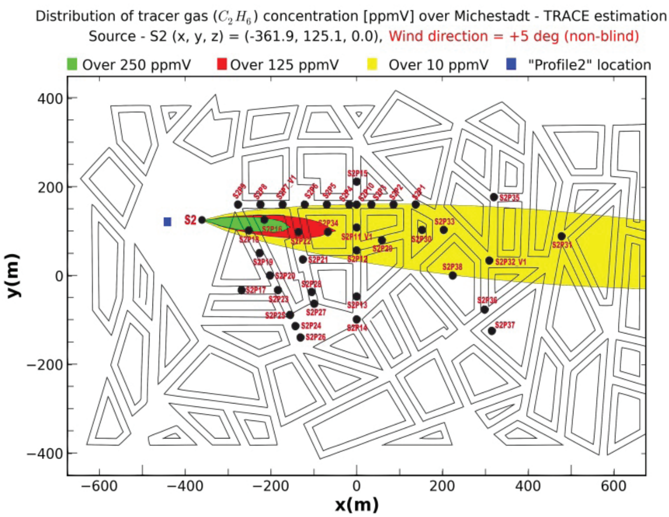


Fig. 5. Wind direction sensitivity of TRACE; top is for 0°; middle for –5°; and bottom for +5°

As seen on Fig. 5 the path of the plume generated by TRACE is slightly wider than the one by ALOHA. On the comparison chart (Fig. 6), however, almost the same pattern of the estimated concentrations is observed. The receptor point S2P9 stays away from the direct influence of the plume, with concentrations of pollutant close to 0 ppmV, and a maximum of the concentration is observed at S2P16 for wind direction 0°. At the latter point, the pollution level estimates for wind directions +5° and -5° are equal, i.e.

we have the same distribution symmetry as with ALOHA. Generally, for the S2 source-receptor set, the best match between measured and estimated concentrations, has the case with the -5° wind direction. It has the highest correlation coefficient (R) (Table 3) and the lowest normalized mean square error (NMSE). Even though the fractional bias (FB) is the highest (-0.47), the difference of its values between the cases is not that big judging by their distance from the ideal value – zero.

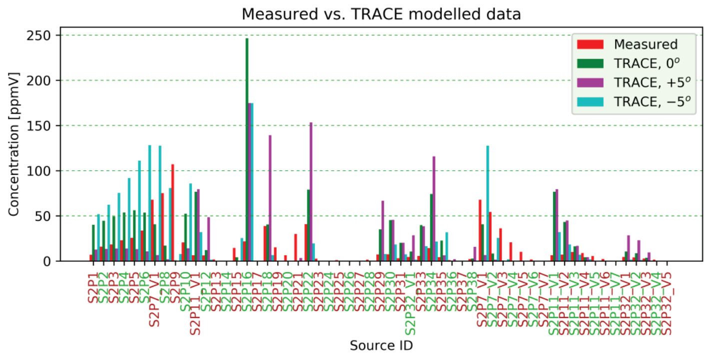


Fig. 6. Comparison between TRACE's estimated (0°, +5° and –5°) and wind tunnel measured concentrations [ppmV] for source S2

Table 3. TRACE statistics for continuous releases

SPM	Wind direction	0°	-5°	+5°
NMSE		4.83	3.77	5.71
R		0.17	0.47	0.09
FB		-0.41	-0.47	-0.35
FAC2 (%)		15.79	12.28	17.54

TRACE provides outputs for dosage and puff duration (ALOHA v5.4.4 provides dosage output only in the version intended for work under the MacOS).

4.3. AERMOD

The surface friction velocity u_* of the wind tunnel's approach flow is calculated from its mean kinematic turbulent flow data and it appears to be 0.566 ms^{-1}. However, over the Michelstadt domain, due to presence of buildings, the surface roughness z_0 and therefore u_* undergo some modifications. As a result, the approach flow vertical wind profile does not correspond to the one observed over Michelstadt. This is the reason for the additional sensitivity tests made with AERMOD for varying values of u_* and z_0 for the urban area.

A picture of the pollution field over Michelstadt according to AERMOD model estimations is shown below (Fig. 7). Since the source of tracer gas is situated at ground level (z = 0.0 m) and the receptor grid flagpole height is 7.5 m, there is a white spot observed at the source location – an absence of pollutant, due to the specifics of the AERMOD concentration distribution, a vertical section of which can be seen on Fig. 8.

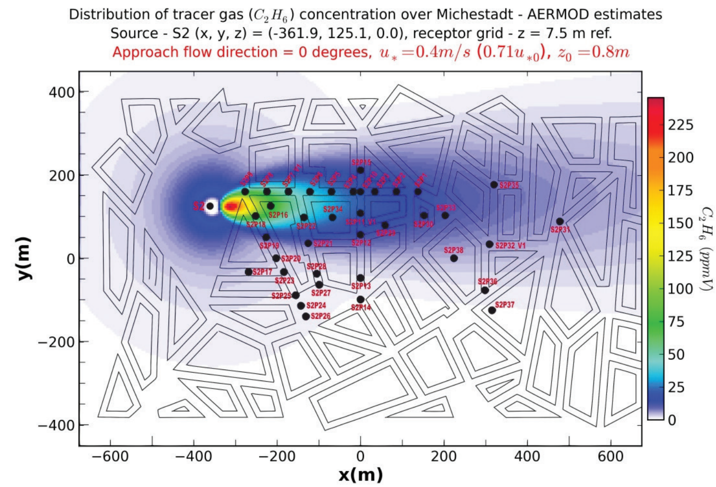


Fig. 7. AERMOD estimated concentration distribution of ethane over Michelstadt

The difference between the pollution distributions modeled by AERMOD and the other two models could be easily noticed. In the represented by AERMOD concentration field on Fig. 7, the pollutant tends not only to spread in the direction of the wind, but to disperse in all directions as well. The drag generated by the surface disturbs and slows down the transport of the pollutant near the ground, resulting in a plume with irregular shape in the vertical plane (Fig. 8). The bar graph (Fig. 9) shows very good match between observed and modeled concentrations, especially for the case with -5° (counter-clock rotated) wind direction, which is as well confirmed by the statistical performance measures (Table 4).

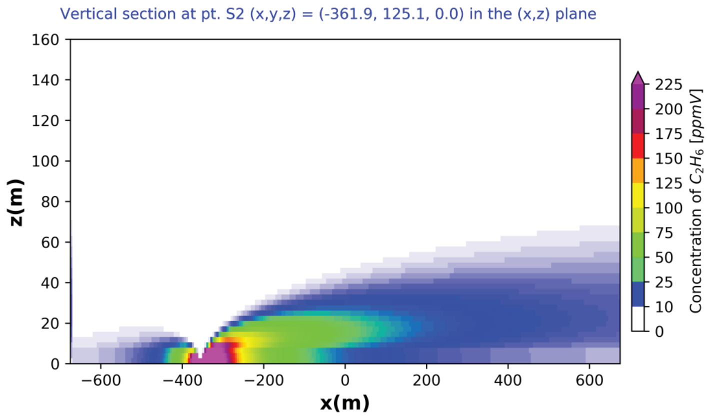


Fig. 8. AERMOD estimated concentration distribution of ethane – a vertical section.

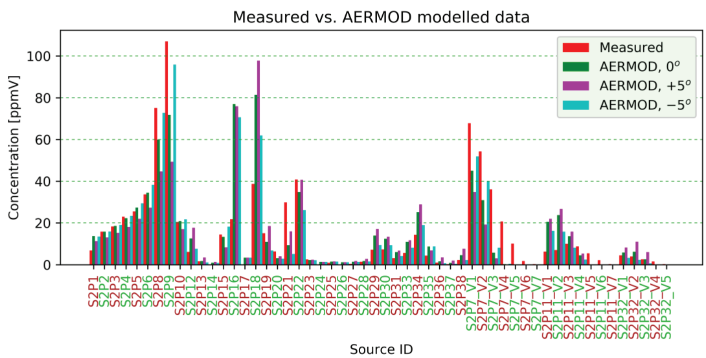


Fig. 9. Comparison between AERMOD's estimated (0°, +5° and –5°) and wind tunnel measured concentrations [ppmV] for source S2

Compared to ALOHA and TRACE AERMOD shows significantly lower sensitivity towards wind direction change. An obvious reason for that could be the wider plume path modeled.

Table 4. AERMOD statistics for continuous releases

SPM	Wind direction	0°	-5°	+5°
NMSE		0.88	0.85	1.45
R		0.76	0.86	0.61
FB		0.01	0.05	0.04
FAC2 (%)		51.85	55.56	40.74

5. CONCLUSIONS.

Gaussian models are still in use despite their simple output. Moreover, some of them are perfected to a degree at which they can be used for urban air pollution modeling where buildings are to some extent taken into account. AERMOD for example has the PRIME algorithm implemented which handles the building downwash effects. ALOHA is designed to calculate the indoor pollution, and handles heavy gas dispersion. Both ALOHA and TRACE include an intuitive user friendly GUI wizard which leads the user step by step to a successful scenario setup in a very short time. From a statistical point of view however, the performance of ALOHA and TRACE confronted with the measured data was very poor. Nevertheless, these two models, with some reservations, could be used as emergency response tools in densely built environments, especially in the cases when they are applied in areas where the count of one to three story buildings is predominant.

AERMOD showed very good results in this particular study. Some GUI wrapped commercial versions of the model could decrease the input data preparation time to an extent at which it could be used as an emergency response model though it is a regulatory one. The open source version of the model armed with the suitable script and batch processing inventory could shrink the preparation time as well.

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