Computational Fluid Dynamics Model to Simulate Methane Dispersion at Oktoberfest

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Abstract

In this paper, a computational fluid dynamics (CFD) model is developed to simulate the methane (CH4) dispersion of exhaust gases from the Munich Oktoberfest, the world's largest folk festival. Since we assume CH4 losses during the natural gas driven heating and cooking process, our aim is to provide a methodology for estimating these emissions. We developed a forward CFD dispersion model and combined it with on-the-site backpack measurements to quantify the emissions at the festival. The emission number is determined by scaling the simulated to the measured concentrations. Our sensitivity study reveals that the turbulent Schmidt number and the measured wind speed have high impacts on the emission results. Further, we investigated the effect of buoyancy, since there is a temperature gradient between the exhaust gases and the environment. Our results show that the buoyancy is an important factor for assessing hot emissions. Finally, we compared our findings to results determined by a Gaussian plume model and discussed advantages and disadvantages of each approach. Our findings show that CFD models can reproduce real dispersion processes in very complex environments with a high spatial resolution and are able to predict emissions. This study offers a completely new methodology to quantify local emissions on a real scale array and presents one of the first attempts to use CFD to study superimposed greenhouse gas sources.

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Key Points: A computational fluid dynamics (CFD) model to simulate the methane dispersion of Oktoberfest was developed. In combination with concentration measurements, the model developed can be used to quantify methane emissions of large area sources. The impact of various input parameters, e.g. turbulent Schmidt number, wind and buoyancy on the results are quantified.

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12 Abstract

In this paper, a computational fluid dynamics (CFD) model is developed to simulate the 13 methane (CH_4) dispersion of exhaust gases from the Munich Oktoberfest, the world's 14 largest folk festival. Since we assume CH_4 losses during the natural gas driven heating 15 and cooking process, our aim is to provide a methodology for estimating these emissions. 16 We developed a forward CFD dispersion model and combined it with on-the-site back-17 pack measurements to quantify the emissions at the festival. The emission number is de-18 termined by scaling the simulated to the measured concentrations. Our sensitivity study 19 reveals that the turbulent Schmidt number and the measured wind speed have high im-20 pacts on the emission results. Further, we investigated the effect of buoyancy, since there 21 is a temperature gradient between the exhaust gases and the environment. Our results 22 show that the buoyancy is an important factor for assessing hot emissions. Finally, we 23 compared our findings to results determined by a Gaussian plume model and discussed 24 advantages and disadvantages of each approach. Our findings show that CFD models 25 can reproduce real dispersion processes in very complex environments with a high spa-26 tial resolution and are able to predict emissions. This study offers a completely new method-27 ology to quantify local emissions on a real scale array and presents one of the first at-28 tempts to use CFD to study superimposed greenhouse gas sources. 29

30 1 Introduction

31 Climate warming is affecting the environment all over the world. Events and changes can be observed which did not occur before. Melting of the ice caps, severe floods, droughts, 32 heat waves and the rising sea level (Bailey & Callery, 2020) are just some examples of 33 possible consequences. A NASA and NOAA analysis (NOAA National Centers for En-34 vironmental Information, 2020) reveals the last decade as the hottest on record and 2019 35 the second warmest year on record. One reason for the present global warming period 36 are the strong greenhouse gas (GHG) emissions. The rate of the rising temperature is 37 unprecedented compared to the past 66 million years (Zeebe et al., 2016). The two most 38 dominant GHGs are carbon dioxide (CO_2) and methane (CH_4) . While CO_2 is already 39 a well-known and widely researched GHG, CH_4 comes more and more in the scientific 40 focus. CH_4 is about 86-times as effective as the same mass amount of CO_2 over a time 41 period of 20 years and 28-times as powerful on a 100 year time scale with respect to its 42 global warming potential (Jackson et al., 2020). In 2007 the CH_4 concentration began 43 to rise after a 7 year period of stagnation (Mikaloff-Fletcher & Schaefer, 2019; Nisbet 44 et al., 2019). Recent studies (Jackson et al., 2020; Saunois et al., 2020) report for the 45 year 2017 a new record high in CH_4 emissions worldwide. CH_4 is responsible for 23 % 46 of the global warming caused by anthropogenic GHGs (Saunois et al., 2020). More than 47 600 million tons of the gas were released to the earth's atmosphere and more than halve 48 of it is caused by human activities according to the authors. While wetlands account for 49 roughly one third of the overall emissions, 20% to 25% each come from agriculture/waste 50 and fossil fuel sources. Further, Plant et al. (2019) and Varon et al. (2019) recently ob-51 served significant CH₄ emissions caused by fossil fuel sources. 52

In order to react and counteract the global warming process, the origin of the GHG plays a key role. When a reduction of emissions is targeted, mainly emissions caused by fossil fuel burning can be tackled, since they are often directly attributable to human activities and can be replaced by alternative processes and techniques. (Nisbet et al., 2020; Ganesan et al., 2019). In order to improve/avoid CH₄ releasing mechanisms and to reduce the impact on climate warming, a model can be built up based on the data gained from possible sources.

This study investigated the largest folk festival of the world, the Munich Oktoberfest. Here, CH_4 emissions are not only a consequence of the high number of visitors, since other possible reasons for unwanted CH_4 release are pipeline leakages and incomplete combustion of natural gas by kitchen appliances and heat generators as indicated by Chen et al. (2020). During the entire festival period in 2019, 185 000 cubic meters of natural gas were consumed (Landeshauptstadt München, 2019). In order to reconstruct the release of fossil CH_4 /natural gas and to quantify possible sources, a model was developed based on CH_4 measurements inside and outside Oktoberfest 2019.

Such models can be based on numerical simulations, relating the exhaust gases of 68 the emission sources and the concentration measurements of the GHGs. For predicting 69 the sources' quantitative impact, Gaussian plume models (Chen et al., 2020) can be used. 70 71 Their results are often very coarse, since no real geometry of the environment is taken into account and the air flow in the region of interest is not simulated. Another approach 72 to obtain emission origins and their behaviour are computational fluid dynamics (CFD) 73 simulations. Here, for creating an appropriate fluid flow model, the spatial resolution of 74 the flow fields is essential. Mesoscale models, such as the Weather Research and Fore-75 casting (WRF) model (Beck et al., 2012; Zhao et al., 2019), work with a grid resolution 76 of about 1 km. In order to analyze emission processes more in detail and to include typ-77 ical GHG sources, such as buildings, power plants, factories and vehicles, the micro-scale 78 approach is more suited. A combination of both scale models is presented by Berchet 79 et al. (2017), who used mesoscale patterns to serve as boundary conditions for a microscale 80 urban flow model. The PALM project (Maronga et al., 2020) also offers urban applica-81 tions of atmospheric boundary-layer flows from meso- to microscale. Since the festival 82 investigated in this paper takes place at a small isolated area of 0.42 km^2 and background 83 measurements are available, we used the mircoscale approach for our simulation model. 84

To provide an overview of the current state of the art in this field, Lateb et al. (2016); 85 Meroney et al. (2016); Tominaga and Stathopoulos (2013) summarized previous projects 86 and milestones. Tominaga and Stathopoulos (2007, 2016); Gromke and Blocken (2015); 87 Yu and Thé (2017); Shi et al. (2008) developed CFD models for simulating pollutant dis-88 persion in urban areas by validating them with wind tunnel data. Idrissi et al. (2018); 89 Wingstedt et al. (2017); Wang et al. (2015) simulated CH_4 and CH_4 based natural gas 90 dispersion in cities by using this method. Simulations based on real geometry are much 91 rarer. A CH_4 emission estimation of a landfill site close to Ipswich (UK) was done by 92 Sonderfeld et al. (2017) using CFD and in situ measurements. Jeanjean et al. (2015); 93 Nozu and Tamura (2012); Van Hooff and Blocken (2010); Patnaik et al. (2007); Hanna 94 et al. (2006) show CFD model approaches in real cities, which are validated by on-site 95 measurements. The only study, which faces the flow of contaminated exhausts emitted 96 by a chimney (up to the authors' knowledge) was done by Toja-Silva et al. (2017). They 97 simulated the CO_2 dispersion from an urban power plant inside the city of Munich (Germany) and validated their findings with on-site measurements. They also analyzed the 99 spatial distribution of CO_2 concentrations by presenting a concentration map. 100

However, the emissions of temporary events such as folk festivals have never been modelled numerically using CFD. This study also offers a completely new methodology to quantify local emissions and presents one of the first attempts to use CFD to investigate superimposed GHG sources on a real scale array.

105 **2** Methodology

In this study a CFD simulation is applied to model the CH_4 dispersion based on CH₄ and wind measurements. Using the measurements and the simulation outcomes, the CH₄ emissions were quantified.

109 2.1 Measurements

As measurement device the LI-COR LI-7810 CH4/CO2/H2O Gas Analyzer was chosen. The gas tracer uses optical feedback-cavity enhanced absorption spectroscopy to analyze the current CH_4 concentration. It captures one sample per second and determines the CH_4 proportion with a precision of 0.25 ppb (5 s averaging) (LI-COR Inc., 2018). Because the instrument has no GPS tracker, a smartphone application was used to record the position of each measurement continuously.

The backpack measurements were split into two different parts: individual surveys inside and outside the festival area. Both are called rounds in the following. For the measurements outside Oktoberfest, the shortest path around the perimeter of the festival premises (Theresienwiese) was chosen. The measurements on Theresienwiese were made following a route, which covered as many potential pollution spots as possible. The route leads through the two main and some side streets (for exact path see Figure C1).

In order to validate measured CH_4 peaks at Oktoberfest, the consideration of wind 122 direction and speed is essential. The exact wind conditions must be also known in or-123 der to set up a CFD simulation, since the fluid flow has to be defined explicitly. For these 124 reasons, the wind measurements were taken as close to the festival as possible, which was 125 a location $150 \,\mathrm{m}$ away from the festival premises. They were recorded on top of a $26 \,\mathrm{m}$ 126 high building, which is located at 48.134188° N and 11.545524° E. The sensor used is 127 a Lufft WS200-UMB 2D ultrasonic anemometer. Since we implement a whole round in 128 the simulation, the wind conditions recorded at a rate of 1 Hz had to be averaged over 129 the time required to complete a round around the perimeter of Oktoberfest. 130

The round, which was investigated in this study, was selected on the basis of the 131 following parameters. The standard deviation of the wind direction and speed should 132 be low, the measured concentration peaks should be clearly visible and the wind direc-133 tion should roughly match the concentration distribution. Further, the measured wind 134 speed of the round should not be below $1.5 \,\mathrm{m\,s^{-1}}$ at dispersion height (which leads to 135 a minimum of $2 \,\mathrm{m \, s^{-1}}$ at wind measurement height). The round, which fitted best to the 136 criteria, was recorded on September 29 at 4:45 pm (UTC). The wind characteristics of 137 this round (mean value \pm standard deviation) are $(240.5 \pm 12.9)^{\circ}$ and $(2.75 \pm 0.91) \,\mathrm{m \, s^{-1}}$. 138

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2.2 Governing Equations of the Fluid Flow

The simulation progress is divided into two steps. First, the wind flow is simulated 140 by the steady-state Reynolds-Averaged Navier-Stokes (RANS) equations, together with 141 a modified standard k- ϵ model (Durbin, 1996). Based on the solved wind field, the CH₄ 142 dispersion is obtained by applying the unsteady convection-diffusion equation. During 143 the wind flow calculation step the exhaust is treated like air, while for the passive-scalar 144 gas transport calculation the exhaust emissions contain a specific amount of CH₄. The 145 model was executed as incompressible first and for the sensitivity study, we also inves-146 tigated the compressible case. All numerical calculations are carried out using the open-147 source software environment OpenFOAM. 148

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2.2.1 Fluid Flow Equations

This study applies the concept of Reynolds. With the RANS equations, larger scale 150 systems can be modelled and the computational cost is the lowest compared to Direct 151 Numerical Simulations (DNS) and Large Eddy Simulations (LES). Besides that, LES sim-152 ulations produce not necessarily better results compared to RANS models, due to high 153 uncertainties of atmospheric models in real urban environments (Patnaik et al., 2007). 154 Therefore, the use of RANS is usually most efficient, when highly accurate results of very 155 turbulent flows are not required (Tominaga & Stathopoulos, 2016). The following sec-156 tion gives a short overview on the theory used in the simulation. 157

¹⁵⁸ On the basis of the well-known Navier-Stokes equations, the expressions for the RANS ¹⁵⁹ were developed. They consist of the momentum equation and the mass conservation (here

in an incompressible form with constant viscosity and density).

$$\rho \frac{\partial \overline{u}_i}{\partial t} + \rho \frac{\partial}{\partial x_j} (\overline{u}_i \overline{u}_j) = -\frac{\partial \overline{p}}{\partial x_i} + \mu \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \rho \frac{\partial}{\partial x_j} (\overline{u'_i u'_j}) \tag{1}$$

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$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{2}$$

where u represents the velocity, p is the air pressure, ρ stands for the air density and μ is dynamic viscosity.

For this project, the turbulence model applied is based on the standard $k - \epsilon$ model. 164 The approach assumes that the flow is fully turbulent and consequently the effects of molec-165 ular viscosity are negligible. On the basis of the standard k- ϵ model, some modifications 166 were made to increase the accuracy. Kato and Launder (1993); Tsuchiva et al. (1997); 167 Yap (1987) made suggestions for improvements, especially tackling the overestimation 168 of the turbulent kinetic energy in the impinging region of bluff bodies. Another approach 169 is the modification of ν_t which is used in our model. Durbin (1996) proposed the calcu-170 lation of ν_t by coupling it to the turbulence time scale T. This approach was developed 171 specifically for simulations with wind flow in urban environments and verified for exhaust 172 dispersion applications by investigating a benchmark case (Toja-Silva et al., 2015). This 173 turbulence model is applied in the following. The values of the coefficients used in the 174 turbulence equations are based on physical experiments. Here the standard values (C_{μ} = 175 0.09, $C_{\epsilon 1} = 1.44$, $C_{\epsilon 2} = 1.92$, $\sigma_k = 1.0$, $\sigma_{\epsilon} = 1.3$) suggested by Pope (2000) 176 are used. 177

2.2.2 Gas Dispersion Equations

The convection-diffusion passive scalar equation for incompressible turbulent flows gives a possible solution for the gas concentration fields. The equation consists of a transient, a convection and a diffusion term.

$$\frac{\partial C}{\partial t} + \frac{\partial \overline{u}_j C}{\partial x_j} - \frac{\partial}{\partial x_j} \left(D_{eff} \frac{\partial C}{\partial x_j} \right) = 0 \tag{3}$$

Here, the volumetric averaged gas concentration is represented by C. $D_{eff} = D + D_t$ is the effective diffusivity. The molecular diffusivity D depends on the kind of gas and the medium surrounding it, and can be found in appropriate literature (Lide, 2004). The eddy diffusivity D_t can be determined by

$$D_t = \frac{\nu_t}{Sc_t} \tag{4}$$

where Sc_t is the turbulent Schmidt number and ν_t represents turbulent viscosity. For 186 pollutant dispersion in environmental flows, Tominaga and Stathopoulos (2007); Blocken 187 et al. (2007); Gualtieri et al. (2017) suggest an acceptable range of 0.1 to 1.0 for Sc_t . Since 188 Sc_t depends on the characteristics of the flow and the location in the flow pattern, it is 189 important where the region of interest is. For plume dispersion downwind and its lon-190 gitudinal transport, small values of Sc_t are suggested by previous studies (Tran et al., 191 2019; Yu & Thé, 2017). These circumstances are given in this study, which is why a small 192 Sc_t is beneficial. Furthermore, trace gas concentrations close to the ground and build-193 ings are better predicted, when a low turbulent Schmidt number compensates a high tur-194 bulent diffusion of momentum, which is often underestimated at these locations (Riddle 195 et al., 2004; Di Sabatino et al., 2007; Blocken et al., 2008; Nakibolu et al., 2009). Espe-196 cially in our case, a high turbulent kinetic energy can be found due to many complex ob-197 stacles which exist on a public festival. Therefore, this study applies a comparatively low 198 Schmidt number of 0.4 as suggested by Yu and Thé (2017), but also investigates the im-199 pact of using different values in the sensitivity study. 200



Figure 1. Numerical simulation geometry as a 16 million cell mesh.

2.3 Numerical Domain and Grid Generation

The geometry model used in this simulation is designed with the CAD tool Au-202 toCAD. Large beer tents (>1000 seats) and buildings on and next to the festival area 203 were constructed in the model. However, since the Oktoberfest geometry is very com-204 plex, not everything was covered precisely by the model. Humans, small booths and var-205 ious fairground rides are hard to model with the given information and a static geom-206 etry. Therefore, a simplified geometry was included for these installations at Oktober-207 fest. The dimensions of the geometries were gathered using satellite images provided by 208 Google, Maxar Technologies. 209

The dimensions of the Cartesian simulation domain are created in OpenFOAM on the basis of the CFD simulation best practice guidelines (Franke et al., 2007). The final model, which includes tents and buildings, has about 16 million cells and is shown in Figure 1.

2.4 Boundary Conditions

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Since RANS equations are used in the CFD model, we applied a velocity-inlet and pressure-outlet for the simulation domain. The remaining boundaries are defined by fixed values, zero gradients and standard wall functions (for an overview of all conditions see Table A1, A2).

At the inlet boundary, where the wind flows into the domain, the measured wind and turbulence conditions are imposed to the model. In order to apply the measured wind speed to the inlet, the equations of Richards and Hoxey (1993) are used. With this approach, the vertical velocity profile, the kinetic energy and the dissipation rate profile of the inlet can be determined. A fixed value is applied for the pressure at the outlet which represents the outflow boundary in the domain.

At the chimney boundaries, a fixed exhaust velocity u_{exh} is applied. It is estimated by the flue-gas stack draft. The relations are derived from Klote (1991). For estimating the flue-gas flow-rate, the molar mass of the exhaust and the surrounding air are assumed to be equal and the frictional resistance and heat losses are negligible.

$$u_{exh} = C \sqrt{2gh \frac{T_i - T_o}{T_i}} \tag{5}$$

The gravity acceleration g is chosen as 9.81 m s^{-2} and h represents the height of the chimney. For the discharge coefficient C, a value of 0.6 is usually assumed. With a chimney height of 6 m and an approximated temperature difference of 80 °C, an exhaust velocity u_{chim} of approximately 3 m s^{-1} is determined. The exhaust temperature is based on

Sadeghzadeh (2007); Dudkiewicz and Szaaski (2020) and selected by considering the cir-233 cumstances in the kitchens, such as heat losses between the devices and the chimney sys-234 tem. Since not every tent has the same guest capacity and thus various amounts of cook-235 ing and heating is done, the different number of available seats have to be taken into ac-236 count. Therefore, the amount of emitted exhausts were modified for every single tent. 237 We assumed that all natural gas fueled devices have the same CH_4 leakage rate and there-238 fore all exhaust flows should have the same CH_4 concentration. If a tent has a higher 239 capacity, more grills and heat generators are suspected. Hence, the outlet flow rises, since 240 the geometry of all chimneys is assumed identical. The average of all outlet velocities 241 is 3 m s^{-1} . For the calculation, all seats inside and outside the tents are considered. 242

For the ground boundary, the sand-grain based fully rough law (Blocken et al., 2007) is used to impose roughness to the boundary surface. The aerodynamic roughness length z_{0} is defined to be 0.2 m and for the roughness constant C_{s} a value of 7 is recommended by Van Hooff and Blocken (2010). This results in a roughness height $k_{s} = 0.2798$ m according to equation 6.

$$k_s = \frac{9.793 \cdot z_0}{C_s} \tag{6}$$

The roughness height of the tents and buildings is set to zero $(k_s = 0)$.

In the second part of the simulation, which simulates the transport and diffusion of CH_4 , the velocity field and the turbulent viscosity are given through the fluid flow simulation and are used as fixed boundary conditions. The background and exhaust concentrations are applied at the boundaries. The determination of the background for the selected round is done by calculating the mean of all concentration values below the 10 % quantile. The exhaust concentration of the chimneys is varied to scale the resulting simulation concentrations to the measurements (see section 2.6).

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2.5 Numerical Procedure and Implementation

The fluid flow simulation of the main model was performed by the incompressible OpenFOAM solver *simpleFOAM* for turbulent flows, which uses the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm to solve the RANS equations. The fluid flow part of the simulation uses Gaussian second order linear interpolation schemes. The residuals for the fluid flow are below 1×10^{-5} .

The diffusion problem is solved by a customized solver *turbulentScalarTransportFoam*, which was previously created by Toja-Silva et al. (2017). It extends the *scalarTransportFoam* solver by including the turbulent eddy dissipation.

The calculations are carried out on the Linux Cluster of the Leibniz Supercomputing Centre (LRZ) on 64 cores in parallel.

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2.6 Determining the Emission Number

In order to determine a total emission number of Oktoberfest, we used the approach 268 as described in Chen et al. (2020) to scale the prior emission number of the forward CFD 269 simulation until the modelled and measured curve match (see Figure 4). For that pur-270 pose, the chimneys' exhaust concentration C_{exh,CH_4} is varied until the areas underneath 271 the measurement and simulation plume curves are equal. Only the measurements out-272 side the Oktoberfest premises were used, as the measurements inside are too much dis-273 torted by local emission sources, such as humans and small booths that we neglected in 274 the model. We considered only the chimneys of the large tents (>1000 seats) as CH₄ emit-275 ters. These chimneys are modelled with an exhaust outflow concentration C_{exh,CH_4} . The 276 mean exhaust velocity of all chimneys u_{exh} is $3 \,\mathrm{m \, s^{-1}}$ and the radius of a single chim-277 ney r_{chim} is 0.3 m. All $n_{chims} = 17$ chimneys have an identical geometry. That infor-278 mation together with the area of Oktoberfest can be used to calculate the overall emis-279

280 sion number:

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$$E = \frac{\rho_{air} \cdot M_{CH_4} \cdot C_{exh,CH_4} \cdot A_{chim} \cdot u_{exh} \cdot n_{chims}}{M_{air} \cdot A_{Oktoberfest}}$$
(7)

where $\rho_{air} = 1204 \,\mathrm{g}\,\mathrm{m}^{-3}$ is the density of air at 20 °C and $M_{air} = 28.94 \,\mathrm{g}\,\mathrm{mol}^{-1}$ represents the molar mass of dry air. $M_{CH_4} = 16.04 \,\mathrm{g}\,\mathrm{mol}^{-1}$ refers to the molar mass of CH₄, while $A_{chim} = 0.28 \,\mathrm{m}^2$ is the cross section area of a single chimney. The part of Theresienwiese, where Oktoberfest takes place, is about $A_{Oktoberfest} = 420\,000 \,\mathrm{m}^2$.

2.7 Sensitivity Study

The simulation model is based on some input parameters, for which no uniform values are suggested in the literature or are not known precisely. For these parameters, a sensitivity analysis was performed to figure out how much variations in these input parameters affect the output.

The choice of the turbulent Schmidt number Sc_t depends on the kind of study and can vary between 0.1 and 1.0 (Tominaga & Stathopoulos, 2007; Blocken et al., 2007; Gualtieri et al., 2017). Based on Yu and Thé (2017), we decided to use 0.4 in this study. However, we ran the simulation also for the numbers 0.2, 0.6 and 0.8 to quantify the uncertainty of choosing a different Schmidt number.

The wind speed and direction fluctuates during a walked measurement round, which took about 35 min. Therefore, the simulations were carried out once using the mean values of the wind speed and direction and two additional times using the wind parameters obtained by subtracting and adding the standard deviation during the measurement round.

The averaged value of the chimneys' exhaust velocities 3 m s^{-1} is estimated on the basis of the exhaust temperatures of the kitchen appliances used (see equation 5). In order to account for the large possible variations in exhaust temperatures, we ran the simulations also for exhaust velocities of 2 m s^{-1} and 4 m s^{-1} .

Since the exhaust gas, which is emitted by the chimneys, has a specific tempera-304 ture, which is significantly higher than the surrounding air, a model considering the buoy-305 ancy effect is developed, too. This simulation consists of a compressible domain, which 306 takes density differences caused by the exhaust temperature into account. When the buoy-307 ancy force is included in the simulation, some modified equations are needed. Usually, 308 two approaches are available for including buoyancy effects to the fluid flow: an incom-309 pressible model with the Boussinesq approximation or a completely compressible model. 310 The Boussinesq approximation could not be implemented, because the simulation is not 311 fulfilling its usage criterion $\beta(T - T_0) \ll 1$. Therefore, the model was simulated as 312 compressible. The pressure term in the momentum conservation equation is replaced by 313 a new parameter p'. Here, p' considers hydrostatic pressure effects. 314

$$p' = p - \rho g z \tag{8}$$

where g is the gravitational acceleration and z the height above the ground. Besides this modification, the energy conservation equation is added, in order to take the exhaust's temperature and therefore the density difference into account. The energy equation is defined as follows:

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$$\frac{\partial(\rho h)}{\partial t} + \nabla(\rho u h) + \frac{\partial(\rho K)}{\partial t} + \nabla(\rho u K) - \frac{\partial p}{\partial t} = \nabla(\alpha_{eff} \nabla h) + \rho u g \tag{9}$$

Here, h stands for the enthalpy and K represents the kinetic energy. The effective thermal diffusivity α_{eff} is the sum of laminar and turbulent thermal diffusivities. The temperature used for calculating the exhaust velocity is also used for the chimneys' temperature boundary, when the simulation is run compressible. The OpenFOAM solver *bouynatSimpleFoam* is applied for the compressible model.



Figure 2. Vertical slice of the flow velocity (left) and the CH₄ concentration (right) at z = 3 m. The chimney outlets are located at z = 9 m.



Figure 3. Isosurface corresponding to C = 1980 ppb. Tent "a"/"b" are marked exemplary for a low/high exhaust velocity u_{exh} .

324 **3** Simulation Results

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This section presents the simulation results and the conclusions of the sensitivity study. Subsequently, a comparison to the Gaussian plume model is shown.

3.1 Concentration Distribution and Emission Number

The vertical wind speed and CH_4 concentration distribution in the domain at 3 m328 height can be seen in Figure 2. There, it is shown that the CH_4 dispersion follows the 329 flow and the concentrations reach the ground right behind the tents. This can be also 330 seen in Figure 3 (for close-up view see Figure B1). The figure shows the plume disper-331 sion in three dimensions and demonstrates that tents with a lower CH_4 outflow veloc-332 ity, such as chimney "a", produce smaller plumes than those with a higher one, such as 333 chimney "b". The concentration distribution on the round around the premises is shown 334 in Figure 4. Here, the unit of the x-axis represents the position on the track around the 335



Figure 4. Measurement and scaled simulation concentration trend on the outside part of the round. The angle defines the position on the outside track $(0^\circ = N; 90^\circ = E)$.

perimeter of Oktoberfest. 0° stands for the point on the round, which intersects a north-336 pointing line from the premises-center. Analogously, 90° is the eastern crossing point on 337 the round. The figure presents the concentration plume curves on the track on ground 338 level of the measurements and the simulation. It can be seen that the plume simulated 339 by the CFD model (brown curve) match the measurements (blue curve) regarding the 340 position on the track and resemble the shape of the measurement plume curve well. Over-341 all, there is a strong correlation between the CFD model result and the outside measure-342 ments as R^2 reaches a values of 0.55 (R=0.74). The resulting emission number is 5.33 µg m⁻² s⁻¹. 343

While the result of the outside round is used to determine the emission number, 344 also concentrations inside the festival area were compared to the measurements. In con-345 trast to the measurements outside the festival area, the result for inside shows less cor-346 relation as $R^2=0.05$ (R=0.22) between the measured and modelled concentrations. Those 347 findings suggest that inside the Oktoberfest area the influence of the chimneys' exhaust 348 is superimposed by small local sources that were not modelled in this study, such as open 349 tent doors and windows, gas heaters in the beer gardens, gas grills in the streets etc. Fur-350 thermore, not all obstacles such as fair rides, small booths and humans are included in 351 the model, which is the reason why the model performs worse for the near field. 352

353 3.2 Sensitivity Study

The input parameters, which can not be precisely determined by relevant literature or measurements, were varied, in order to analyze their impact on the result. Table 1 summarizes the parameters, which are used for the uncertainty assessment and shows their impact on the emission number.

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3.2.1 Turbulent Schmidt number

Besides the chosen value of of 0.4 for the turbulent Schmidt number, the resulting plume curves for the values 0.2, 0.6 and 0.8 can be seen in Figure 5 (top-left). It is visible that the absolute concentration values are highly dependent on the choice of the turbulent Schmidt number. A higher Sc_t leads also to higher concentrations on ground level. This means that increasing the value will reduce therefore the emission number and vice versa. The emission number is therefore significantly dependent on the turbulent Schmidt number.

As pointed out in section 2.2.2, the Schmidt number depends on the observing position in the flow. For locations downwind, where CH_4 is transported longitudinal, low numbers are suggested (Tran et al., 2019; Yu & Thé, 2017). Further, close to the ground



Figure 5. CH_4 concentration distribution for different turbulent Schmidt numbers (up-left), different mean chimney exhaust velocities (up-right), the measured wind speed (bottom-left) and wind direction (bottom-right) with its standard deviation. All cases use an exhaust concentration of $C_{exh} = 191 \text{ ppm } (0^\circ = \text{N}; 90^\circ = \text{E}).$

and buildings, a small Sc_t compensates the turbulent diffusion of momentum, which is 369 often underestimated at these locations (Riddle et al., 2004; Di Sabatino et al., 2007; Blocken 370 et al., 2008; Nakibolu et al., 2009). Since this is given in our case, a Schmidt number lower 371 than standard values around 0.7 is reasonable. On the other hand, decreasing Sc_t affects 372 the spatial dispersion of the trace gas (see Figure 5, top-left). The distribution is more 373 uniform and local peaks get damped. In this study, the selection of 0.4 is a good com-374 promise between capturing the spatial distribution and properly approximating the tur-375 bulent kinetic energy at the ground. 376

3.2.2 Wind Speed and Direction

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The wind speed and direction measurements have a mean value and a standard de-378 viation of (2.75 ± 0.91) m s⁻¹ and $(240.5 \pm 12.9)^{\circ}$. The impact of the wind fluctuations, 379 when the standard deviations are applied each, can be seen in Figure 5 (bottom). Gen-380 erally, the effect of changing wind direction on the simulation results is very dependent 381 on the geometry and level of direction fluctuations. For this investigation, the main part 382 of the plume is slightly shifted. However, the overall concentration level stays similar and 383 thus also the area underneath the plume curve. Therefore, the wind direction has only 384 a limited impact on the emission prediction process (up to 4%) in this case. 385

When the wind speed rises, the resulting CH_4 concentration at ground level decreases and as a result the emission number increases proportionally. The wind speed and emission number are therefore positively linearly correlated. Besides the turbulent Schmidt number, the wind speed is essential for assessing source emissions and should be measured carefully.



Figure 6. CH₄ concentration distribution with (compressible) and without (incompressible) the buoyancy effect with $C_{exh} = 191 \text{ ppm} (0^{\circ} = \text{N}; 90^{\circ} = \text{E}).$

Table 1. Uncertainties and their effect on the emission number (EN).

Type	Value	Deviation	Effect on EN
Turb. Schmidt number	0.4	+/-0.2	-27%/+77%
Wind speed	$2.75\mathrm{ms^{-1}}$	$+/-0.91{\rm ms^{-1}}$	+33%/-33%
Wind direction	240.5°	$+/- 12.9^{\circ}$	+2%/-4%
Chimney exhaust velocity	$3\mathrm{ms^{-1}}$	$+/-1{ m ms^{-1}}$	$-0.6\%/{+1.1\%}$

391 3.2.3 Exhaust Velocity

Figure 5 (top-right) shows the concentration distribution with a u_{exh} of $2 \,\mathrm{m \, s^{-1}}$, 392 $3 \,\mathrm{m\,s^{-1}}$ (default) and $4 \,\mathrm{m\,s^{-1}}$. The qualitative CH₄ dispersion shape for the three vari-393 ation cases does not change. However, it is clearly visible that the averaged exhaust ve-394 locity has a quantitative impact on the resulting CH_4 concentration magnitude. The higher 395 u_{exh} is, the higher the simulated concentrations at ground level. As a result the exhaust 396 CH_4 concentration of the chimneys has to decrease for the simulated ground concentra-397 tions to match the measured ones. However, the effect on the emission number is lim-398 ited, since the emission number is calculated by equation 7, where the lower exhaust con-399 centrations are compensated by the increase of u_{exh} . Therefore, the impact on the pre-400 dicted number stays at about 1%. This means that for emission predicting purposes, u_{exh} 401 does not play a key role. However, if the absolute concentration magnitude is the result 402 of interest, the exhaust velocity has a significant impact. 403

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3.2.4 Compressible Approach

In order to understand if and how the emission number is changed by taking the 405 temperature differences between exhaust and the surrounding air into account, we com-406 puted the case again, considering buoyancy. For the compressible approach, an air den-407 sity gradient is allowed in the domain. Figure 6 shows that this approach has a signif-408 icant impact on the results. Considering buoyancy, the gas stream is lifted upwards, which 409 results in a lower concentration at the ground. Therefore, the emission number rises due 410 to the higher chimney exhaust concentration, which is needed to compensate that effect. 411 Numerically, the effect causes an increase of the emission number from 5.33 to $7.24 \,\mu g \, m^{-2} \, s^{-1}$ 412 (+36%).413



Figure 7. Comparison of scaled results by CFD and Gaussian plume (GP) models for the outside round $(0^\circ = N; 90^\circ = E)$.

3.3 Comparison to Gaussian Plume Model

While the CFD simulation of the exhaust flow of Oktoberfest was done for the first 415 time in this study, a Gaussian plume model was already developed for the Oktoberfest 416 investigation in 2018 (Chen et al., 2020). The Gaussian plume model is a steady-state 417 approach, which simulates the transport of gas emissions and the diffusion released by 418 a point source. The dispersion is represented by a plume which fits the concentration 419 distributions to Gaussian curves in vertical and horizontal directions (Pasquill, 1966, 1969, 420 1979; Gifford, 1976; Briggs, 1973; Hanna et al., 1982). The results of the two different 421 modeling approaches are compared. In 2018, an average emission number of $(6.7 \pm 0.6) \,\mu g \, m^{-2} \, s^{-1}$ 422 was determined. The emission number found by the present study using CFD and con-423 sidering buoyancy, is $7.24 \,\mu \mathrm{g} \, \mathrm{m}^{-2} \, \mathrm{s}^{-1}$, which is within the uncertainty range of the num-424 ber determined in 2018 using the Gaussian plume model. We conclude that both Gaus-425 sian plume and CFD simulations are suitable for emission estimates of area sources us-426 ing the approach presented in Chen et al. (2020). 427

Figure 7 shows scaled simulated plume curves on the basis of a CFD simulation 428 and the Gaussian plume model, which was applied using the setup of Chen et al. (2020). 429 Figure 7 shows that there exists a difference in the shape of the two plumes. While the 430 CFD simulation captures more details, such as single peaks, the Gaussian Plume model 431 represents a low-pass filtered version of the signal. We conclude that for investigations, 432 where a high spatial resolutions is needed, the CFD model offers the possibility to re-433 produce local enhancements in a greater detail. Such a feature is especially helpful to 434 predict concentrations at a certain point or to inversely model emissions using station-435 ary sensors. Gaussian plume models, by contrast, can provide the overall distribution 436 well, which is sufficient to determine the emission number based on mobile measurements. 437 Furthermore, the calculation effort for the Gaussian plume model is significantly less. 438 439

440 4 Conclusion

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This article presents a CFD model, simulating CH_4 dispersions in a complex urban environment. For the first time, a large folk festival, in this case the Munich Oktoberfest, was investigated using fluid dynamics simulations with a spatial resolution of 2 m in the regions of interest.

Based on the results of Chen et al. (2020), the big tents are assumed to be the largest CH₄ emitters. For this reason, a CFD model of Oktoberfest was set up, defining the chim-

⁴⁴⁷ neys of each tent as CH_4 sources. Using a RANS model, the dispersion of the gas is sim-⁴⁴⁸ ulated. In order to validate the simulation results and determine the emissions, CH_4 con-⁴⁴⁹ centration measurements with a mobile CH_4 backpack analyzer around and inside Ok-⁴⁵⁰ toberfest were carried out, too.

The modelled CH_4 concentrations were scaled to the measurements outside Ok-451 toberfest by varying a prior emission number. The result shows that the simulation case 452 match the overall CH_4 distribution shape of the outside measurement round well. Es-453 pecially, the qualitative allocation of the CH_4 peaks is similar to the distribution of the 454 455 measurement maxima. However, the modelled concentration distribution inside the festival area looks different compared to the measured values. We suspect local turbulence 456 and additional CH_4 sources (e.g. humans, food stands), which are not considered in the 457 model, to be the reasons. In our case, the CFD model reconstructed downwind concen-458 trations well (R=0.74), but for near-field applications the result was inadequate (R=0.22). 459

The resulting emission number of the incompressible case is $5.33 \,\mu g \,m^{-2} \,s^{-1}$. When the buoyancy force is considered in the model, the CFD emission number increases, since the CH₄ plume is lifted upwards resulting in lower concentrations at ground level. In this case the emission number rises to $7.24 \,\mu g \,m^{-2} \,s^{-1}$ (+36%). This number is in the same magnitude as the value found by Chen et al. (2020) using a Gaussian plume model (6.7 $\pm 0.6 \,\mu g \,m^{-2} \,s^{-1}$).

In order to determine how certain the calculated emission number is, we performed 466 a sensitivity study on all decisive input parameters of the model, such as turbulent Schmidt 467 number, wind speed and direction and the exhaust velocity. The turbulent Schmidt num-468 ber Sc_t has a significant impact on the emissions and simulated concentration distribu-469 tions. There exists a negative correlation between Sc_t and the emission number, since 470 an increasing Schmidt number leads to a higher longitudinal plume spread. In this study, 471 a value of 0.4 was used for Sc_t . A 50% higher Schmidt number, leads to a emission num-472 ber decrease of 27%. The wind speed is linearly correlated to the emission number. Chang-473 ing the wind speed by its standard deviation leads to a $\pm 33\%$ emission number change. 474 The chimneys' exhaust velocity has only an influence on the absolute concentration mag-475 nitude, not on the resulting emission number, as an exhaust velocity variation cancels 476 out with the resulting exhaust concentration change when calculating the emissions. 477

This study shows, how CH_4 concentrations of a complex urban domain, such as Ok-478 toberfest, can be successfully modelled using a spatially highly resolved CFD model. In 479 future studies, it could be beneficial to take more gas sources into account, since the tents' 480 chimneys are not the only emitters of CH_4 as identified by our on-site investigations. Only 481 then, it will be possible to model the near field, i.e. concentrations inside of the premises, 482 accurately. This can be done by extending the geometry and adding surface sources. In 483 addition, LES modelling can be used for simulating dispersed gas of multiple chimney 484 sources in order to compare LES with RANS models regarding the applicability in such 485 complex real urban environments. 486

Conclusively, this study shows that CFD is a powerful tool for simulating high-resolution
atmospheric GHG dispersion caused by multiple trace gas sources in a complex urban
domain. In combination with concentration measurements, it can be used to quantify
local emissions and estimate the overall impact of these sources to the environment. The
advantages of CFD simulation compared to the Gaussian plume model are the very high
spatial resolution which can be used to forecast concentrations at specific locations and
the possibility to predict emissions using just a few stationary sensor sites.

Table A1. Fluid flow boundary conditions imposed at each boundary of the domain (incompressible model). Nomenclature: Cc = Calculated, fV = fixedValue, iV = inlet value, sl = slip, wF = wall function, zG = zeroGradient.

	U	k	ϵ	$ u_t$	р
Inlet	iV	iV	iV	\mathbf{Cc}	zG
Outlet	zG	zG	zG	Cc	fV zero
Ground	fV zero	kqR wF	epsilon wF	nutk rough wF	zG
Buildings	fV zero	kqR wF	epsilon wF	nutk wF	zG
Chimneys	iV	iV	iV	Cc	zG
Sky	sl	sl	sl	Cc	\mathbf{sl}
Sides	sl	sl	sl	sl	\mathbf{sl}

Table A2. Dispersion boundary conditions imposed at each boundary of the domain. Nomen-clature: Cc = Calculated, fV = fixedValue, iV = inlet value, sl = slip, zG = zeroGradient.

	u	$ u_t$	\mathbf{C}
Inlet	fV	\mathbf{Cc}	iV
Outlet	fV	$\mathbf{C}\mathbf{c}$	zG
Ground	fV	fV	zG
Buildings	fV	fV	zG
Chimneys	fV	$\mathbf{C}\mathbf{c}$	iV
Sky	fV	$\mathbf{C}\mathbf{c}$	zG
Sides	fV	sl	zG



Figure B1. Closer look to the "Schützen" and the "Paulaner" tent.



Figure C1. Spatial distribution of measured and simulated CH_4 concentrations outside and inside the Oktoberfest premises with wind direction (arrow) and chimney positions (points). Map provided by Google, Maxar Technologies.

494	Appendix A	Boundary	Conditions
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- ⁴⁹⁵ Appendix B Close-up View on Chimneys
- Appendix C Heatmaps of the measured and simulated CH₄ Concentrations
- 498 Acronyms
- ⁴⁹⁹ **CFD** Computational Fluid Dynamics
- 500 **DNS** Direct Numerical Simulation
- 501 GHG Greenhouse Gas
- ⁵⁰² **LES** Large Eddy Simulation
- 503 **RANS** Reynolds-Averaged Navier-Stokes
- ⁵⁰⁴ **SIMPLE** Semi-implicit Method for Pressure Linked Equations

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