MEMO²: MEthane goes MObile – MEasurements and MOdelling

New tools to estimate CH_4 source strengths from point sources, including mobile measurements

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Deliverable D.3.1			
Delivery month Annex I	24		
Actual delivery month	24		
Lead participant: WUR	Work package: 3	Nature: report	Dissemination level: public
Version: 1			

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 722479.

Table of content

1. Executive Summary

The MicroHH model (van Heerwaarden et al., 2017) is a Computational Fluid Dynamics (CFD) code for the simulation of turbulent flows. Our MicroHH simulation code has been further developed and improved towards our actual model requirements. It is adapted in order to simulate emissions from point and line sources of methane from arbitrary positions in the domain. Special boundary conditions were developed to allow for free outflow of methane, while maintaining circular boundary conditions for the flow. The source is added in the form of a 3D Gaussian function over four standard deviations to prevent numerical artefacts that would arise if the mass was inserted into a single grid cell. The boundary has been adapted to satisfy Neumann boundary condition on the right boundary and Dirichlet condition on the left. These adaptations to the code now allow for long simulations of methane dispersion from point and line sources. This, in turn, allows for extensive statistical studies of dispersion in a fully resolved turbulent flow.

The new "CH_4-plume"-enabled MicroHH tool facilitates future research on turbulent dispersion not only in simplified conditions, but also in complex terrain, such as for instance the surroundings of a farm, or a landfill. Moreover, simulations can be used to improve measurement strategies and more accurate estimations of methane sources, including characterization of errors.

2. Introduction

2.1 Background

Mobile measurements of methane plumes are normally conducted in the planetary boundary layer (PBL), part of the atmosphere close to the Earth's surface, where the behavior of measured methane plumes is dictated by the turbulent nature of the flow. Due to the stochastic nature of turbulence this strongly influences the interpretation of the measured values. The most commonly used models for dispersion of pollutants are of the Gaussian plume model type. These models are computationally very cheap, which makes them attractive to use, but they are highly empirical, and difficult to adapt to weather, landscape elements that disrupt the flow, and are only able to capture the average dynamics of turbulent plumes. This makes them unsuitable for direct interpretation of short-duration concentration measurements in a turbulent field. Large-eddy simulations (LES) or direct numerical simulations (DNS), which resolve turbulence, give full turbulent behavior of the plumes, but are computationally expensive. Another option is the use of Reynolds-averaged Navier Stokes (RANS) equations. In theory, RANS simulations represent an ensemble average of turbulence resolving models, which makes them capable of quantifying mean transport. However, their capabilities in capturing turbulent fluctuations are limited.

The MicroHH model (van Heerwaarden et al., 2017), which will be described here, is a Computational Fluid Dynamics (CFD) code for the simulation of turbulent flows. The model is designed for DNS but also supports LES. It is written in C++ and CUDA. The model solves equations of conservation of mass, momentum and energy under the Boussinesq or inelastic approximation. The time integration is performed with Runge-Kutta integration schemes of either third-order or fourth-order. Spatial discretization is on a staggered Arakawa C-grid, which places the scalars in the center of a grid cell and the velocity components on the faces.

2.2 Scope of the deliverable

The MicroHH model will be used for the simulation of dispersion patterns from different sources of methane (point, line, diffuse) under various meteorological conditions and over surfaces with different heterogeneities and surface roughness. This new tool is intended for the interpretation of the short-duration methane observations close to methane sources in different circumstances, and should allow for reliable source strength estimation.

3. Content

The existing MicroHH code has been adapted to enable the simulation of multiple point and line sources of methane at arbitrary positions in the domain. To avoid possible numerical artefacts that would arise from injecting mass into a single grid point, the point sources have been added in the form of a 3D Gaussian over four standard deviations (σ_i, i= x, y, z) around the source location (x_0, y_0, z_0). Defined this way, the source S, has the shape:

$$S = Qa \times exp\left(\frac{-(x-x_0)^2}{\sigma_x} - \frac{(y-y_0)^2}{\sigma_y} - \frac{(z-z_0)^2}{\sigma_z}\right).$$

Here Q is the source strength in kg / s and a is a normalization constant defined in a way that the Gaussians integrate to Q.

The boundary conditions in the code have also been adapted such that the outflow of the scalar on the right boundary was set using Neumann boundary condition:

$$\left.\frac{\partial f(x,y,z)}{\partial x}\right|_{x_r} = const.$$

where x_r is the position of the right boundary. Similar applied for the left boundary, there the Dirichlet condition was set: $f(x,y,z)_{x_l} = const.$ where x_l is the position of the left boundary.

The result of a standard simulation with the adapted MicroHH code is displayed in Fig. 1, which is a snapshot of a simulation of a methane release in the PBL from an elevated point source and over a flat terrain. The simulation follows the case study by Moser et al (1999) of a simple channel flow.

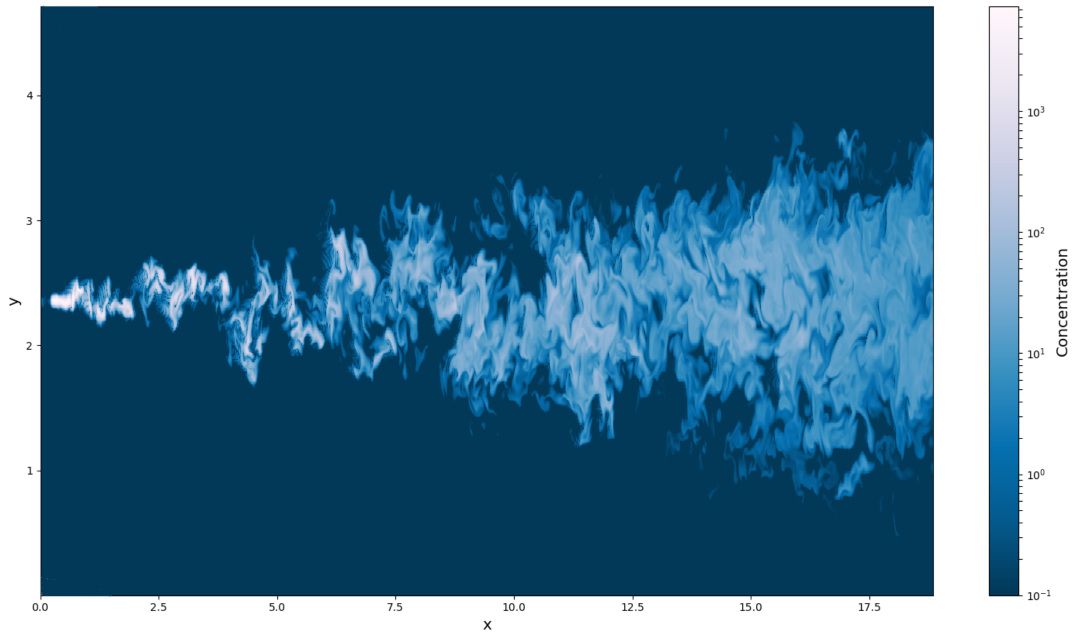

Fig.1: Example of a high-resolution simulation of an elevated point source release in MicroHH.

Using this standard simulation, different measuring techniques can be tested and evaluated as well as the simpler models that simulate dispersion in the atmosphere, for example the Gaussian plume model. For illustration, in Fig. 2 multiple transects through the plume are shown.

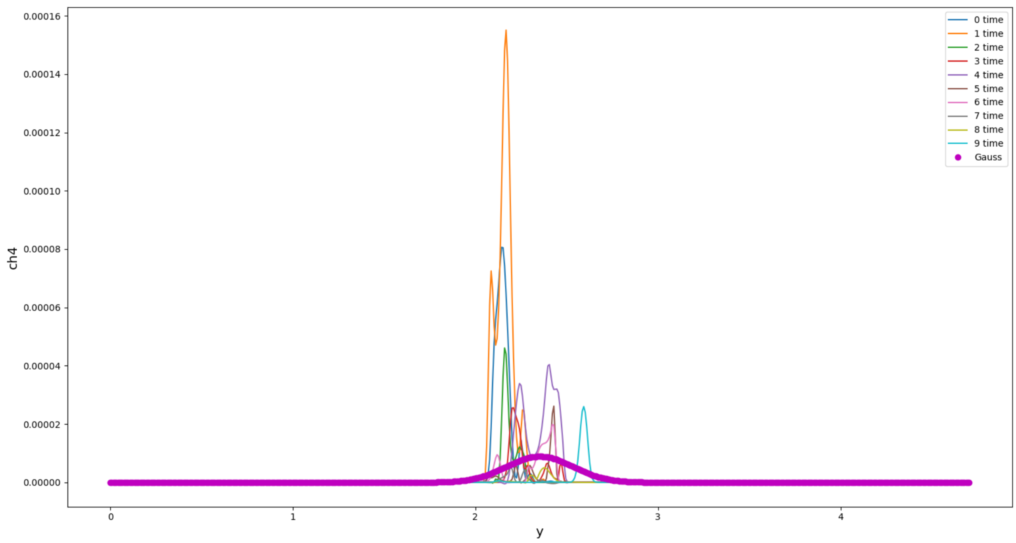

Fig. 2: Multiple plume transects through the plume centerline, taken from the DNS run. Superimposed over is a transect from a Gaussian plume model for the same conditions.

Transects are taken instantaneous, perpendicular to the main wind, and at the plume centerline. Also, the transects are taken at ten consecutive seconds (i.e. with different dispersion characteristics). This situation resembles mobile measurements with e.g. a car, with the difference that here we observe the whole plume at a single moment and have the exact wind values at each point of the domain. This enables us to study the effects of the turbulence on the plume dispersion more accurately. Superimposed over the transect is the result from a Gaussian plume model that corresponds to the simulation performed in MicroHH, meaning that the source strengths in the models are the same and the wind value corresponds to the mean wind at the height of the plume centerline averaged over the whole DNS domain in the horizontal direction. As can be observed in Fig. 2, concentration transects are significantly different from one time step to the next. Differences are visible in the value of concentrations (typically much higher in DNS) as well as the spatial distribution. Obviously – and by definition - the Gaussian plume model is not capable of capturing this variability, and if a Gaussian plume would be fitted to a single plume transect (i.e. a measurement transect) this would lead to a significant misinterpretation of the measurements. This is already showing the importance of multiple plume measurements and averaging, since in theory the Gaussian plume represents the average of an infinite number transects. Further studies will focus on

- the evaluation of different plume sampling methods and optimal averaging transects.
- non-instantaneous sampling (has already been implemented)
- back-calculation of the source strength, depending in sampling strategy
- evaluation of real measurement data, using statistical approaches
- dispersion simulations over complex terrain

4. Conclusion and possible impact

The new "CH_4-plume"-enabled MicroHH tool facilitates future research on turbulent dispersion not only in simplified conditions, but also in complex terrain, such as for instance the surroundings of a farm, or a landfill. Moreover, simulations can be used to improve measurement strategies and more accurate estimations of methane sources, including characterization of errors.

5. Dissemination & Exploitation

The code is open source and is available on GitHub (www.microhh.org). In collaboration with MEMO²-partner Shell, measurement techniques are already being evaluated.

6. References

1. Moser, R.D., Kim, J., Mansour, N.N. (1999): Direct numerical simulation of turbulent channel flow up to Re(τ)=590. Physics of fluids, Vol.11, No.4, 943-945.

2. Van Heerwaarden, C., van Stratum, B. J. H., Heus, T., Gibbs, J.A., Fedorovich E., Mellado, J.P. (2017): MicroHH 1.0: A computational fluid dynamics code for direct numerical simulation and large-eddy simulation of atmospheric boundary layer flows. Geosci. Model Dev.

7. History of the document

7.1 Document history

Version	Author(s)	Date	Changes
Beta 1	Anja Raznjevic, Chiel van Heerwaarden	12 Feb 2019	
Beta 2	Maarten Krol	20 Feb 2019	Track changes

7.2 Internal review history

Internal Reviewer	Date	Comments
Sylvia (Beta 1)	21 Feb 2019	Track changes, email
Sylvia (Beta 2)	06 March 2019	Final formatting