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Integration of OpenFOAM Flow Simulation and Filament-Based Gas Propagation Models for Gas Dispersion Simulation

Sepideh Pashami, Sahar Asadi, Achim Lilienthal
Centre of Applied Autonomous Sensor Systems,
Örebro University, Sweden
{sepideh.pashami, sahar.asadi, achim.lilienthal}@oru.se
http://www.aass.oru.se/

Abstract
In this paper, we present a gas dispersal simulation package which integrates OpenFOAM flow simulation and a filament-based gas propagation model to simulate gas dispersion for compressible flows with a realistic turbulence model. Gas dispersal simulation can be useful for many applications. In this paper, we focus on the evaluation of statistical gas distribution models. Simulated data offer several advantages for this purpose, including the availability of ground truth information, repetition of experiments with the exact same constraints and that intricate issue which come with using real gas sensors can be avoided.
Apart from simulation results obtained in a simulated wind tunnel (designed to be equivalent to its real-world counterpart), we present initial results with time-independent and time-dependent statistical modelling approaches applied to simulated and real-world data.

Keywords Gas dispersion, CFD, OpenFOAM.

1 Introduction

Gas distribution modelling has important applications in industry, science, and every-day life. Air pollution monitoring is required for long-term assessment of air quality and to support immediate measures in case of hazardous chemical incidents, for example. Of particular interest in our research work are data-driven, statistical gas distribution models, which can provide comprehensive information about a large number of gas concentration measurements, highlighting, for example, areas of unusual gas accumulation. Such models can also help to locate gas sources and to plan where future measurements should be carried out.
Evaluation of gas distribution modelling approaches requires a sufficient number of sample measurements over a certain period of time and reliable ground truth information. Due to the difficulty to collect concentration measurements and the respective ground truth data in real-world experiments, it is very important to complement real-world measurements with data from realistic gas dispersal simulation. Apart from the availability of ground truth information, simulations of gas dispersal have additional advantages: they enable repetition of experiments under identical conditions, relatively effortless testing in various scenarios, and avoid intricate calibration issues, which typically occur with gas sensors used in dense sensor networks.
In this paper, we present a gas dispersal simulation package that integrates OpenFOAM fluid flow simulation [3] and the filament-based gas propagation model introduced in [2]. Different flow models available in OpenFOAM can be used. In this paper, we present results obtained under the assumption of compressible flows. The filament-based gas propagation model implements an efficient plume model. The simulation package will be published as open

source software.
In the following, the theory behind the gas dispersal simulation is first sketched in two parts: the governing equations of the turbulent flow model (Sec. 2.1) and the gas propagation model (Sec. 2.2). The implemented gas dispersal simulation method is detailed in Sec. 3. That is modelling fluid flow with OpenFOAM and the filament-based gas propagation models are explained. Finally, snapshots of simulated gas dispersal are presented and the derived data-driven statistical gas distribution models are shown (Sec. 4). The paper ends with a summary and a discussion of future work (Sec. 5).

2 Theory

In this section, we discuss the governing equations for modelling compressible flow (Sec. 2.1) and the propagation of gas in filaments (Sec. 2.2). A basic assumption we make is that the flow affects gas propagation but gas propagation does not affect the flow. Any numeric simulation of fluid dynamics must satisfy conservation equations: conservation of mass, momentum and energy. In the following we specifically discuss the conservation of mass in a filament-based dispersion model as it is used in our implementation.

2.1 Turbulent Flow Models

Turbulent flow models are mostly based on Reynolds Averaged Navier-Stokes (RANS) equations, which can be classified as either eddy-viscosity or Reynolds stress models. Fluid flows can be either laminar, in transition from laminar to turbulent or fully turbulent. Different turbulence models can be used in order to model a turbulent flow. Sklavounos and Rigas [4] showed that a good agreement between simulated and measured gas dispersion can be achieved using a k-ε turbulence model (an eddy-viscosity model). We chose the k-ω-SST turbulence model instead in order to avoid the necessity to employ damping functions and a strong sensitivity to the free-stream value of ω [5]. The k-ω-SST formulation switches to a k-ε behavior in the free-stream. Generally, the gas dispersal package presented here is independent of the turbulence model and different models can be used.
The k-ω-SST turbulence model is a two-equation eddy-viscosity model described by the following equations:
kinematic eddy viscosity,

$$\nu_T = \frac{a_1 k}{\max(a_1 \omega, S\, F_2)} \tag{1}$$

turbulence kinetic energy,

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \beta^* k\omega + \frac{\partial}{\partial x_j}\left[(\nu + \sigma_k \nu_T) \frac{\partial k}{\partial x_j} \right] \tag{2}$$

specific dissipation rate,

$$\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha S^2 - \beta \omega^2 + \frac{\partial}{\partial x_j}\left[(\nu + \sigma_\omega \nu_T) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1)\sigma_{\omega 2} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_i} \tag{3}$$

with closure coefficients $(F_2, P_k, F_1, CD_{k\omega})$ defined as follows:

$$F_2 = \tanh\left(\left[\max\left(\frac{2\sqrt{k}}{\beta^* \omega y}, \frac{500\nu}{y^2 \omega}\right)\right]^2\right) \tag{4}$$

$$P_k = \min\left(\tau_{ij}\frac{\partial U_i}{\partial x_j}, 10\beta^* k\omega\right) \tag{5}$$

$$F_1 = \left\{\left\{\min\left(\max\left(\frac{\sqrt{k}}{\beta^* \omega y}, \frac{500\nu}{y^2 \omega}\right), \frac{4\sigma_{\omega 2} k}{CD_{k\omega} y^2}\right)\right\}^4\right\} \tag{6}$$

$$\mathrm{CD}_{k\omega} = \max\left(2\rho\sigma_{\omega 2}\frac{1}{\omega}\frac{\partial k}{\partial x_i}\frac{\partial \omega}{\partial x_i}, 10^{-10}\right) \tag{7}$$

In Eq. 1 the parameter is set to $a_1 = 0.31$ and S is the SST model strain rate. The model constants are calculated using the closure coefficient F_1 function

$$\phi = \phi_1 F_1 + \phi_2 (1 - F_1) \tag{8}$$

The parameters α, β, σ_k and σ_ω are calculated based on the Eq. 8 by replacing ϕ with the respective parameters. The parameter values used in Eq. 2-7, were selected as in the standard k-ω-SST model:

$$\alpha_1 = \frac{5}{9}, \alpha_2 = 0.44, \beta_1 = \frac{3}{40}, \beta_2 = 0.0828, \beta^* = \frac{9}{100},$$
$$\sigma_{k1} = 0.85, \sigma_{k2} = 1, \sigma_{\omega 1} = 0.5, \sigma_{\omega 2} = 0.856.$$

2.2 Gas propagation model

The complex interaction of gas with its surrounding is typically dominated by three physical effects. First, on a long time scale, molecular diffusion mixes the gas with the surrounding atmosphere to achieve a homogeneous mixture of both in the long run. Second, turbulent air flow fragments the gas emanating from a source into intermittent patches of high concentration with steep gradients at their edges [6]. Third, flow advectively moves these patches. Due to the effects of turbulence and advection of flow, it is possible to observe high concentrations in locations distant from the source location.

The filament-based dispersion model we propose in this paper takes into account all three effects mentioned above. Gas is represented by a sequence of puffs and each puff is composed of a number of filaments. The filaments are gas patches with a predefined spherical shape. A chemical released at a source location is affected by turbulent and molecular diffusion along its path while being transported by advection with the wind. Taking into account molecular diffusion and advection, the new position of every filament is calculated based on

$$\dot{p} = v_a + v_m \tag{9}$$

where, $\dot{p}$ is the change of the filament center location per time unit, v_a represents advection and v_m represents the intermediate range of scales that transport filaments within the body of the plume. In our implementation, we obtain v_a from OpenFOAM and v_m by sampling from a Gaussian distribution.

Turbulent diffusion is used to calculate the concentration and changing size of the filament. At every position **x**=(*x*,*y*,*z*), the concentration at time *t* is calculated as sum over the concentrations at that location contributed by each filament

$$C(x,t)=\sum_{i=1}^{N} C_i(x,t) \tag{10}$$

where *N* is the number of filaments currently being simulated. The unit of the concentration is $\frac{molecules}{cm^3}$ and each filament *i* contributes

$$C_i(x,t)=\frac{Q}{R_{i,t}^3}\exp\left(\frac{\left|x-p_{i,t}\right|}{R_{i,t}^2}\right) \tag{11}$$

to the concentration. The parameter *Q* represents the number of molecules per filament, $R_{i,t}$ is a parameter controlling the width (see also Eq. 15), and $p_{i,t}$ is the current position of the *i*-th filament. The value of the $R_{i,t}$ increases over time. In our implementation, the filament growth is defined by Eq. 15.

According to Eq. 11, the concentration of each filament decays exponentially with increasing distance from its centre. Integrating the concentration of the *i*-th filament over the (infinite) spatial extent of the filament gives the number *Q* of molecules in the filament. Mass is conserved as the filament size $R_{i,t}$ changes.

For simulation of the measurements process, the sensed concentration at each gas sensor position is modelled as the thresholded, low pass filtered instantaneous concentration according to the differential equation:

$$\frac{d\,c(t)}{dt}=-\lambda c(t)+\lambda C(x_s(t)) \tag{12}$$

where λ is the filter bandwidth, *c(t)* is the internal state of the filter (its current response), and $x_s(t)$ is the (possibly time varying) sensor position. The input to the filter is the instantaneous concentration at the sensor location $C(x_s(t))$. Using the sensor threshold ξ the output value *y(t)* at time *t* and position $x_s(t)$ is computed as

$$y(t)=\begin{cases} c(t) \text{ if } c(t) > \xi, \\ 0 \text{ otherwise.} \end{cases} \tag{13}$$

An alternative way to the gas dispersal simulation proposed in this paper is to simulate the movement of gas particles directly with OpenFOAM. To decrease the computational demands, sets of physical particles are abstracted into computational particles, which are called parcels. All physical particles within a parcel are assumed to have the same properties.

The movement of the parcels is computed by the Langrangian solver and Gaussian noise is added after each time step. The parcels are similar to the filaments in a filament-based model, however, the size of a parcel does not change over time. Accordingly the effect of diffusion onto the shape of gas patches is not modelled.

3 Filament-Based Gas Dispersion Model

The implementation of the proposed gas dispersal simulation method is divided into two parts: flow simulation with OpenFOAM and a filament model.

3.1 OpenFOAM Flow Model

OpenFOAM is an open source CFD simulation tool, which numerically solves the governing equations of fluid flow. It offers different CFD algorithms to model laminar or turbulent flow. Like with other CFD tools, flow simulation in OpenFOAM includes three steps: a pre-processing step, the actual solver and visualization of the results. The pre-processing step consists of the definition of the environment, including to specify the geometry in the form of a mesh.

Geometry and mesh have been designed by the gmesh tools (BlockMesh could also be used). Designed geometries cover the environment, that is the walls, obstacles, inlets and outlets. Designing a mesh also includes choosing the mesh type (for instance hexahedral) and grid refinement through a grid generation process.

For visualization we use ParaView, which is an open-source visualization application provided with OpenFOAM.

The solver can be chosen from the available OpenFOAM solvers. Currently, OpenFOAM has thirteen sets of solvers. We prefer a compressible flow model in order to model all possible future phenomena in the air flow field. A list of suitable solvers for our purpose is presented below [3]:

- rhoCentralFoam: Density-based compressible flow solver based on central-upwind schemes of Kurganov and Tadmor.
- rhoSimpleFoam: Steady-state, semi-Implicit Method for Pressure-Linked Equations (SIMPLE) solver for laminar or turbulent Reynold Averaged Navier-Stokes (RANS) flow of compressible fluids.
- rhoPisoFoam: Transient Pressure-implicit Split-Operator (PISO) solver for compressible, laminar or turbulent flows.
- rhoPimpleFoam: Transient solver for laminar or turbulent flow in compressible fluids for Heating, Ventilating, and Air Conditioning (HVAC) and similar applications (merged PISO-SIMPLE).

The initial conditions required to be set are the same for all these solvers, so they can be used interchangeably. Each of these solvers can apply either an eddy-viscosity or a Reynolds stress model. Computational cost of the Reynolds stress models is higher compared to Eddy-viscosity models. In the developed simulation package an Eddy-viscosity model is applied.

3.2 Filament-based Gas Dispersion

In the developed gas dispersal simulation package, gas propagation is modelled using the filament-based approach introduced by Farrell et al. [2] in a time- and memory-efficient way. Gas is simulated as a set of filaments (i = 0, . . . , N), each containing a constant amount of molecules or particles $Q = 8.3 \times 10^9$. Filaments are defined by their position, $p_{i,t}$ and width, $R_{i,t}$.

In each time step t, the position of every filament is updated according to the wind flow $v_{p_{i,t}}$ and a stochastic process:

$$p_{i,\Delta t} = p_{i,t} + v_{p_{i,t}} \Delta t + \varepsilon_p \tag{14}$$

where $v_{p_{i,t}}$ is the wind vector at position $p_{i,t}$ .The stochastic component ε_p is a vector of three independent Gaussian random variables, $N(0, \sigma_p^2)$, with standard deviation $\sigma_p = 0.1$ m.

To model molecular diffusion, filaments become wider with time while their peak concentration decreases. The width of a filament evolves as

$$R_{i,t+\Delta t} = R_{i,t} + \frac{\gamma}{2R_{i,t}} \tag{15}$$

with $\gamma = 4 \times 10^{-7}$.

Although all the gas dispersal simulation is generally implemented in 3D, the implemented visualization tool for odour propagation is 2D. The visualization is implemented using OpenGL.

4 Results

This section presents results obtained with the proposed simulation package simulating gas dispersal in a wind tunnel. The wind tunnel environment was selected to match available data from experiments at the DISAL lab, EPFL, Lausanne. The original experiments were carried out at room temperature with largely laminar airflow (approximately 1m/s). A single gas source was located at the position (1m,1.5m) from the bottom left corner of the 16×4 m^2 wind tunnel. The measurements were collected with a metal oxide sensor mounted on a Cartesian robot arm. Accordingly, the simulation environment is a rectangular area of 16×4 m^2 and the thermo-physical properties chosen are those of air at room temperature. In all trials, there is one outlet located at one end of the tunnel. The gas source releases 100 filaments per second with an initial width of $R_{i,0}$ = 0.1 m and an initial position which is uniformly distributed over the circular area of the source. An example simulation in which an obstacle was placed in the tunnel is illustrated in Fig. 1. For the experiment shown in Fig. 1, the rhoPisoFoam solver with the k-ω-SST turbulence model was used. Flow intensity and direction are shown in the top and middle of the Fig.1, respectively. The snapshot at the bottom (Fig. 1) illustrates the gas dispersion model created by the proposed filament-based simulation.

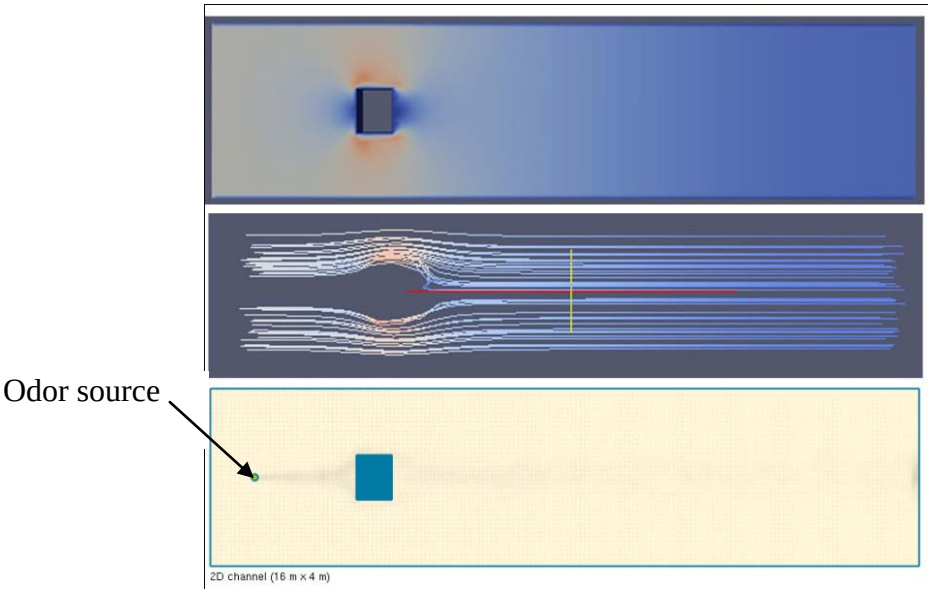

Figure 1: Gas dispersion simulation: Flow intensity (top,) flow direction (middle) and snap shot of the gas dispersal model (bottom). The colors in the top and middle panel represent the flow velocity (increasing velocity from blue to orange).

4.1 Evaluation of Statistical Gas Distribution Models by Gas Dispersal Simulation Data and Real Measurements Data

For the challenging task of building gas distribution models from a set of spatially and temporally distributed gas sensor measurements we use statistical modelling methods. A statistical approach to gas distribution modelling treats gas sensor measurements as random variables and tries to find a truthful statistical representation of the observed gas distribution from a set of localized measurements. One aim is to provide comprehensive information

about a large number of gas sensor measurements, highlighting, for example, areas of unusual gas accumulation. A statistical gas distribution model can also help to locate gas sources and to plan where future measurements should be carried out.
The gas dispersal simulation proposed in this paper provides valuable input to evaluate alternative approaches to gas distribution modelling not least because they come with ground truth knowledge.
Here, we use the Kernel DM+V method by Lilienthal et al. [1], which estimates the predictive distribution mean and variance over a discretised grid. In Sec. 4.2, we also apply an extension of Kernel DM+V that considers the recency of measurements (compared to a time-scale that can be set or learned from the data) in order to compute the distribution model.
Fig. 2 shows a comparison of the statistical gas distribution model obtained by applying Kernel DM+V to either the data from real measurements collected in the wind tunnel experiment or to simulated data obtained with the proposed filament-based approach. In both cases, the collection of data was started sufficiently long after the source was activated so that the gas distribution reached a steady state. Fig. 2 shows the distribution model from the real sensor data in the top panels and the distribution model from the simulated data in the bottom panels. The distribution models are shown as the predictive mean (on the left) and the predictive variance (on the right), respectively.
The general similarity between the models is visible but there are also noticeable differences. First, the plume shape is not exactly aligned with the tunnel in the real experiment. This is a characteristic feature that was observed in many experiments in the wind tunnel. Second, the variance map is rather different with the maximum of the variance map closer and more clearly localized around the location of the gas source. In this respect it is important that the data in the real experiment were collected over several hours in which the robot arm traversed the whole wind tunnel. Since the gas sensors are to some degree sensitive to temperature and humidity, the map also reflects variations in these parameters, which can undergo substantial changes over the long measurement duration. Third, the mean map created for the simulation experiment shows higher values close to the source location. It is not straightforward to explain this observation. Generally the gradient along a plume is shallow. Small changes in the sensitivity of the sensors around a certain time during the measurement process, eventually caused by varying environmental parameters, could therefore be responsible for the very different location of the peak in the mean distributions.

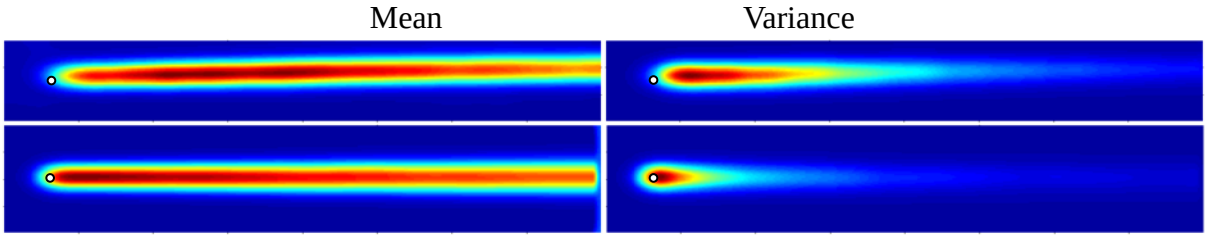

Figure 2: Predictive mean (left) and variance (right) obtained with Kernel DM+V for real experimental data (top), and simulated data (bottom). The source locations are indicated by the white circles.

4.2 Gas Dispersal Simulation for Evaluation of Statistical time-dependent Gas Distribution Models

Kernel DM+V estimates the average gas distribution under the assumption that the distribution is generated by a time-independent random process. While this assumption is valid under certain circumstances, it is also clear that a random process that can change over time is generally desirable. If the assumption of a time-independent random process is not valid, younger measurements should intuitively have a bigger influence on the created model.

This is implemented using recency-weighting in the time-dependent extension of the Kernel DM+V algorithm (TD Kernel DM+V). Since the proposed simulation package can be used to generate snapshots of the evolution of a gas plume, we can use the simulated data also to evaluate TD Kernel DM+V.

Fig. 3 shows consecutive snapshots over a period of 4 seconds taken from the simulation of gas dispersion in the wind tunnel. The evolution is also visible in the corresponding models, i.e. the predictive mean (left) and variance (right) obtained using TD Kernel DM+V. First results of this ongoing work also show that the time-dependent extensions are more accurate compared to the time-independent models in terms of the predictive likelihood of unseen measurements.

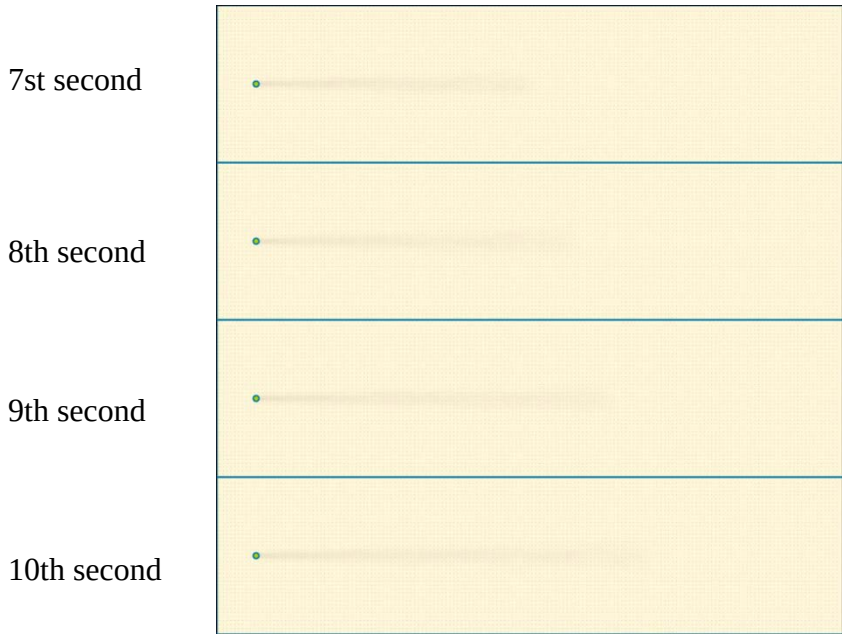

Figure 3: Consecutive snapshots of gas dispersion simulated over a period of 4 seconds.

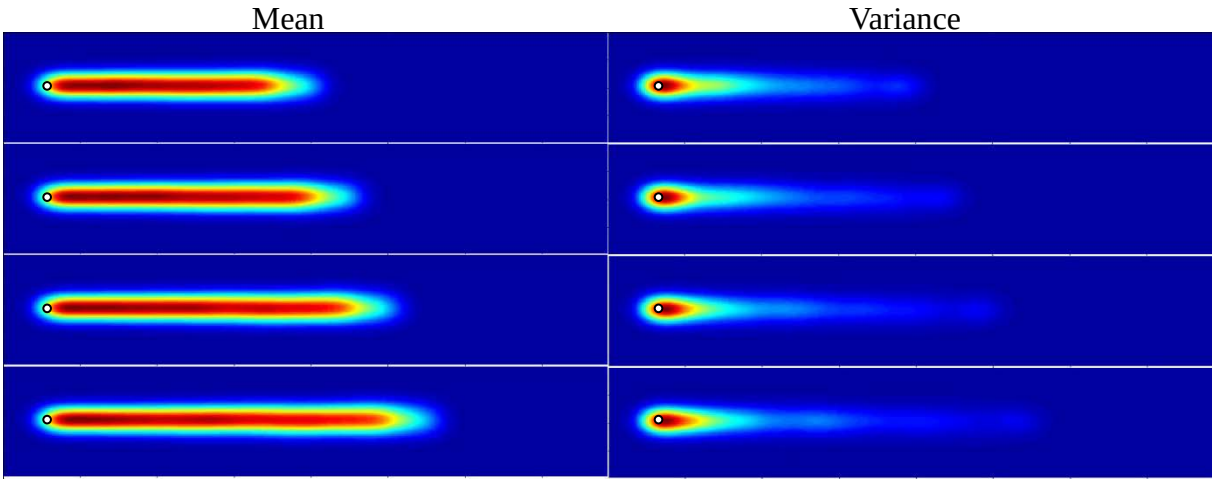

Figure 4: Predictive mean (left) and variance (right) obtained with TD Kernel DM+V for simulated data corresponding to the simulation snapshots shown in Figure 3 (from top to bottom). The source locations are indicated by the white circles.

5 Summary and Conclusions

In this paper, we present a gas dispersal simulation package which integrates OpenFOAM flow simulation and the filament-based gas propagation model by Farrell et al. [2] to simulate gas dispersion for compressible flows with a realistic turbulence model. Gas dispersal simulation can be useful for many applications and it is therefore intended to publish the

presented gas dispersal simulation package as open source software.
Our main interest, which leads to the development of the gas dispersal simulation package, was the evaluation of statistical gas distribution models. Simulated data offer several advantages for this purpose, including the availability of ground truth information, repetition of experiments with the exact same constraints and that intricate issue which come with using real gas sensors can be avoided.
Apart from simulation results obtained in a simulated wind tunnel (designed to be equivalent to its real-world counterpart), we present initial results with time-independent and time-dependent statistical modelling approaches applied to simulated and real-world data. These results are meant to highlight the importance of the proposed simulation package. They currently do not allow to draw final conclusions about the statistical gas distribution modelling methods used.
Apart from a more extensive evaluation of different statistical gas distribution modelling approaches, the simulation package will also be used in the near future to evaluate sensor planning methods and different temporal and spatial sampling approaches. We are further going to extend the visualization of gas dispersion to three dimensions and consider integration of the gas dispersion package with a robot simulation tool.

6 Acknowledgments

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