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# Comparing Different Methods for Calculating the Gas Dispersion

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When handling flammable and/or toxic liquids or gases, the gas dispersion following a release of substance is a scenario to be considered in the risk assessment to determine the lower flammability distance (LFD) and toxicity thresholds. In this work a comparison of different gas dispersion tools of varying complexity ranging from a simple Gaussian model over a boundary layer model (BLM) and a Lagrangian model to CFD (in this case ANSYS CFX v14) is presented. The BLM covers the special case of liquid releases with formation of a pool. It does not only solve the gas dispersion but also calculates the evaporating mass flow out of the pool. The simulation values are compared to each other and to experimental data resulting mainly from our own open air experiments covering the near field and carried out on the Test Site Technical Safety of BAM (BAM-TTS) for different release types (pool evaporation, gas release) and topologies. Other validation data were taken from literature and cover large scale experiments in the range of several 100 m.

## 1. Introduction

CFD methods are used more and more for risk assessment purposes and are especially promising in the field of atmospheric dispersion of pollutants, e.g. flammable and / or toxic gases, fumes etc. They allow to set all kind of obstacles and boundary conditions for the analysis of transient three dimensional phenomena and therefore are rather powerful compared to more analytical or empirical solutions. In the literature a lot of publications can be found dealing with the CFD simulation of gas dispersions (Labosky&Jelemensky, 2011; Kisa&Jelemensky, 2009; Luketa-Hanlin et al., 2007; Rigas&Sklavounos, 2006). Nevertheless, a comparably high number of publications deal with open questions when using CFD for atmospheric flows (Blocken et al., 2007; Franke et al., 2004; Miles&Westbury, 2003). For example, a Gaussian dispersion model does not require a special knowledge of the wind field as it assumes a power law profile, whereas CFD results strongly depend on the wind field assumed. Besides these restrictions, CFD is costly, time consuming and requires expert knowledge. Simpler models are often not designed for providing any 3D information or to account for specific boundary conditions but at least they are mostly quick and easy to use compared to CFD.

In this work the German VDI Guideline 3783, Part 1 (1987) for neutral and light gas dispersion based on a Gaussian approach and Part 2 (1990) heavy gas dispersion based on wind tunnel experiments, a Lagrangian dispersion model as used in AUSTAL 2000 (Austal, 2012; Janicke&Janicke, 2003) and a BLM (Habib, 2011) are compared with simulations with ANSYS CFX v14.0.

In order to give an estimation of the quality of each of the different approaches, open air gas dispersion experiments have been carried out at the BAM-TTS. During these tests gas releases were investigated as well as the gas dispersion from an evaporating liquid pool. For the latter case a specific BLM was developed in order to directly solve the evaporating mass flow and the subsequent gas dispersion in the vicinity of the pool. The results of these smaller scale experiments which cover the near field dispersion with dispersion ranges of several meters, as well as literature data from large scale test series as for example the Prairie Grass test runs (Barad, 1958) with ranges of several 100 meters were used for comparison and validation of the applied models.

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## 2. Theoretical background

### 2.1 VDI Guideline 3783, Part 1 and 2

The German Guideline 3783 (1987,1990) is widely used and accepted for hazard assessment in Germany. Especially for land use planning in the context of DIRECTIVE 2012/18/EU (Seveso III) it is established as a standard calculation tool. The guideline distinguishes between heavy and light gas dispersion. Part 2 (1990) of the guideline defines the density required for a gas to be considered as “heavy”. Furthermore, heavy gas dispersion has to be considered only if the released volume or volumetric flow exceeds a certain threshold.

The heavy gas dispersion as described in Part 2 of the guideline is based on results that have been obtained in systematic wind tunnel experiments. Dimensional analysis can be used to transfer results obtained using small-scale models directly to realistic release amounts and environmental conditions. The Guideline contains further information on dimensional analysis and on the assumptions and simplifications applied. If the concentration of the (heavy) gas cloud is close to or below 1 Vol.%, the guideline assumes that heavy gas effects will be negligible and the transition to light gas dispersion is reached. Especially for toxic gases concentrations below 1 Vol.% are still relevant, so that Part 1 and 2 must be coupled when releasing a heavy gas.

The light gas dispersion model described in Part 1 (1987) of the guideline is based on a Gaussian dispersion model. It is assumed that the centre point of a released gas cloud is transported at a constant wind speed. Mixing with air causes the cloud to be continually diluted, leading to an increase in volume. This process of dispersion and dilution of the cloud as a result of turbulent diffusion is represented by the “dispersion parameter” in the Gaussian model. These dispersion parameters have been measured in experimental investigations over a range of 100 m to 10,000 m. Hence, a restriction of this approach is that considerations for distances below 100 m are subject to significant inaccuracies.

### 2.2 Lagrangian Model AUSTAL 2000

AUSTAL2000 (Austal, 2012; Janicke&Janicke, 2003) is a freely available atmospheric dispersion model based on a Lagrangian particle model for simulating the dispersion of air pollutants in the ambient atmosphere. It is described in VDI Guideline 3945, Part 3 (2000) and although not named in the TA Luft, it is the reference dispersion model accepted as being in compliance with the requirements of Annex 3 of the TA Luft and the pertinent VDI Guidelines. The gas dispersion is computed by virtually releasing point like particles which travel with the calculated wind field. The gas concentrations in each cell of the calculation mesh are determined by integrating the number of particles in the cell at every moment in time. AUSTAL is able to account for turbulence, building effects, terrain influence but is limited to the dispersion of neutrally buoyant or light gases. Especially the fact that buildings can be represented correctly and taken into account makes AUSTAL2000 an interesting alternative to CFD. It promises comparable results with much less time and hardware requirements.

### 2.3 Pool evaporation / Boundary layer model

Up to now, empirical models (e.g. Mackay/Matsugu, Sutton/Pasquill, etc.) have generally been used to estimate mass flow rates of evaporation. The latter are then used as input parameters for a gas dispersion model as for example the VDI Guideline 3783. Based on the two dimensional boundary layer equations coupled with an algebraic turbulence model, the BLM, involving an acceptable level of computational effort, allows for a more accurate and sophisticated calculation of the evaporating mass flow as well as the calculation of the subsequent gas dispersion in the near field of the source. Due to its two dimensional formulation a significant over-prediction of the concentration in the far field will occur. Being developed with special focus on pool evaporation, only area sources can adequately be represented.

The calculations with the VDI Guideline 3783, AUSTAL2000 and the BLM were carried out using the commercial software package for numerical hazard simulation ProNuSs (Pronuss, 2012).

### 2.4 ANSYS CFX v14.0

The commercial CFD code CFX utilizes the Reynolds averaged Navier-Stokes equations for calculating the momentum, heat and mass transfer. Additional mathematical models are used to account for the turbulence. In this work the k-ε turbulence model was used, on the one hand because, apart from its relative simplicity, it has proven to achieve good agreement with experimental results (Sklavounos & Rigas, 2006; Scargiali et al.,2005; Kisa & Jelemensky, 2009) and on the other hand it offers the possibility to easily adapt the turbulence parameters k and ε to the measured wind and turbulence profiles. This allows to overcome the problems occurring when simulating an atmospheric boundary layer flow with CFX as described by Blocken et al. (2007). Richards and Hoxey (1993) and Labovsky and Jelemensky (2011) describe how the turbulent kinetic energy and the eddy dissipation rate can be derived from the friction velocity u* from the log-law wind profile. For the simulations with CFX the Values of u* measured during the experiments were taken to set up an appropriate k-ε level in the simulation domain. The simulations were carried out on Meshes refined to the extent that further refinement would not influence the results significantly. The simulations were mostly carried out as transient runs. Only for simulation of Literature data stationary runs were used, because no transient information on the boundary conditions were available. The simulations were carried out with the ground of the domain set as a smooth, no slip "Wall" boundary condition and all other surfaces set as "Opening" boundary conditions with the wind profile and the k-ε parameters defined on them. Buoyancy was activated and the heat transfer was solved using the "Thermal Energy" model of CFX (ANSYS, 2011).

## 3. Experiments

Our own open air experiments comprised 3 different sets of experiments. All experiments were carried out using R134a (1,1,1,2-Tetrafluoroethane) as gas. According to the definition of the VDI Guideline 3783, Part 2 R134a is a heavy gas. Consequently, heavy gas effects are to be expected at least close to the source. The first experimental setup is using a porous hose laying on the ground in a flat terrain without obstacles and covering circular areas of 1, 2 and 3 m in diameter in which the gas was released. These experiments were simulating a liquid pool with evaporating liquid. The mass flow for these experiments was set to 6 g/s corresponding to calculations of the evaporating mass flow with the BLM for real liquid R134a pools. The second setup comprised a point source in a flat terrain with no obstacles and a mass flow of 55 g/s R134a. The third experimental setup comprised the same point source located directly next to a cylindrical obstacle (dimensions: 5 m Diameter, 4 m Height). For all experiments the wind speed, wind direction and turbulence parameters were measured using an ultrasonic anemometer. The temperature and relative humidity were recorded as well as the transient mass flow rate. The gas concentrations close to the source with values of several Vol.% were measured with Oxygen sensors of the type Draeger Polytron 7000 and further form the source, where the concentrations are in the range of ppm, with sensors of the type FIGARO TGS 832.

Furthermore data of the Prairie Grass trials, as published in literature, were used. During these trials $SO_2$ was released as a tracer gas in a total of 68 runs. The release occurred from a point source 0.46 m over the ground and the measuring points were located on arcs in the distances of 50, 100, 200, 400 and 800 m.

## 4. Results and Discussion

### 4.1 Area source / Pool evaporation

Figure 1 shows the experimental values from the gas dispersion with a mass flow of 6 g/s R134a out of an area source with 2 m diameter in comparison with the results of the BLM and transient CFX calculations. Both models show good agreement with the experimental results. The BLM values tend to over predict the experimental values with increasing distance to the source due to the two dimensional formulation. Therefore no lateral dispersion is occurring and the concentration can only decrease by vertical dispersion. The higher over prediction of CFX and the BLM from 1 m distance is certainly due to the change of sensor type. Below 1 m the oxygen sensors with a good reaction time were used and beyond 1 m the Figaro sensors with a much longer reaction time were used. Due to the continuous wind direction changes a maximum concentration moving back and forth will probably not be detected by the sensors. On the other hand the wind measurements were done upstream of the source so that the real wind field downstream is unknown, leading to differences between the simulated wind fields and the experimental ones resulting in these concentration differences. Nevertheless, both CFX and the BLM predict values in a very close range to each other and in fair agreement with the measured values, over predicting them by a maximum factor of approximately 5.

### 4.2 Point source on flat terrain and close to an obstacle

Figure 2 shows the experimental values of a release of 55 g/s R134a through a point source in a flat terrain without obstacles. In addition the figure shows the results of a stationary and a transient CFX run. Both runs were set up with k-ε parameters and the wind field adapted to the measured u* values. Similar to Figure 1, a different slope of the experimental values is noticeable between the oxygen (0 to 6 m) and the Figaro sensors (9 to 15 m). The figure clearly shows that the representation of a highly transient phenomenon like open air gas dispersion cannot be reproduced satisfactory by a stationary simulation. The CFX values of the stationary run neither match the experimental values nor do they show a similar trend. In contrast to that, the transient run which accounts for the measured (upstream) wind, temperature and mass flow changes during the experiments, gives a much better appreciation of the concentrations.

Although an over prediction by a maximum factor of around 10 is obtained, the transient simulation still provides satisfying results.
During the experiment wind rotation of 180° partially pushed the cloud back in direction of the source resulting in locally higher concentrations than for a stationary plume. The stationary run ignores changes in the wind direction, causing an underestimation of the concentrations close to the source whilst this phenomenon is well represented by the transient run.

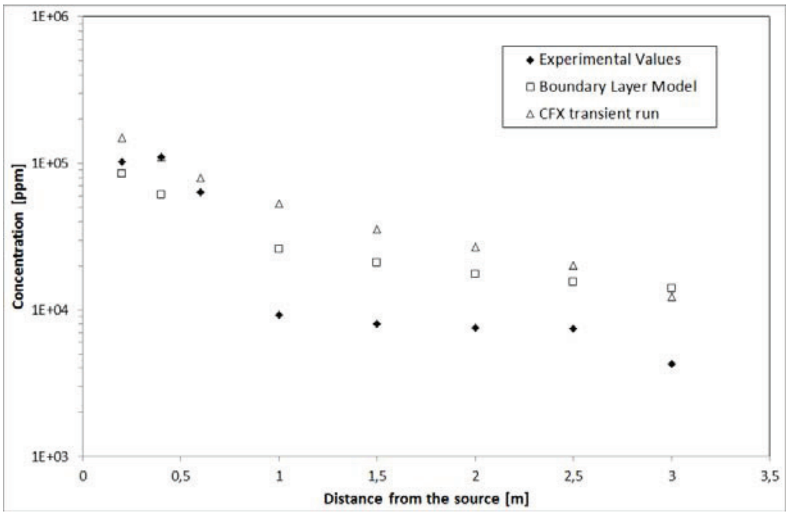

*Figure 1: Comparison of the maximum values of the experimental results, the BLM and transient CFX run for a 2 m diameter area source with a mass flow of 6 g/s R134a*

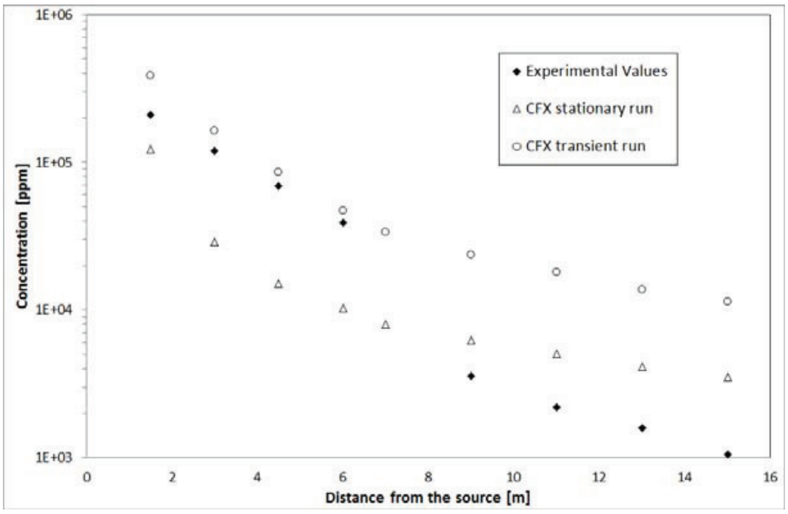

*Figure 2: Comparison of CFX calculations with the experimental results of a gas release out of a point source with a mass flow of 55 g/s R134a*

Figure 3 shows the measured and the simulated concentrations of a point source release with 55 g/s R134a near an obstacle for all 8 oxygen and 40 Figaro sensor locations. Although the obstacle induces much more turbulence, the CFX results show that this is well represented in the simulation. Although an increasing over prediction with increasing distance can be observed, the measured and simulated values differ only by a maximum factor of approximately 10.

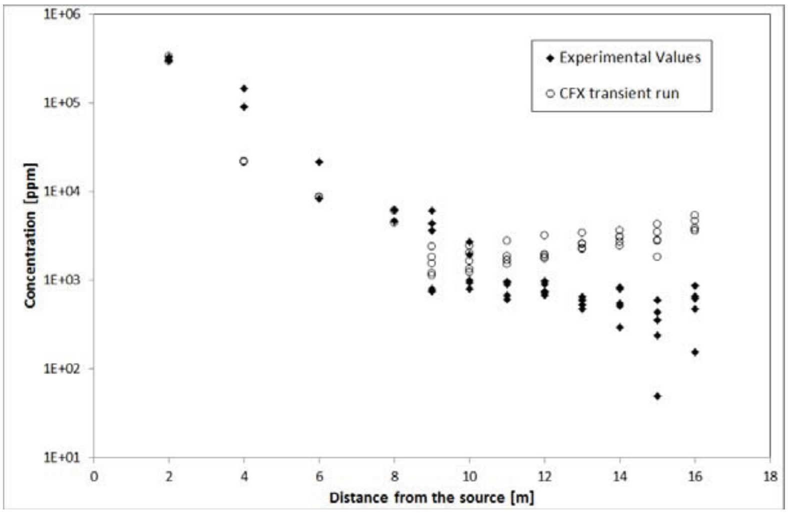

*Figure 3: Measured and CFX simulated concentrations for a release of 55 g/s R134a out of a point source close to a cylindrical obstacle of 5 m diameter and 4 m height*

### 4.3 Large scale gas dispersion

Figure 4 shows the comparison of the Prairie Grass runs Nr. 10 and 36 with the results of CFX, the VDI Guideline 3783 and AUSTAL2000. As there were no transient data available, the simulations were carried out as steady state runs. It has to be noted that AUSTAL2000 shows a very good agreement with the experiments for both runs, while CFX only matches run Nr. 36 with a comparable quality, whereas the VDI Guideline constantly under predicts the experimental values. The main difference between both runs is that run Nr. 10 occurred under a Pasquill-Gifford stability class of B (unstable) and Nr. 36 under a class of F (very sable). Whilst AUSTAL200 can directly account for the stability classes, CFX would need the specific turbulence parameters and the wind field. As there was only a mean wind speed available, all calculations with CFX were carried out with the same turbulence settings. The VDI Guideline seems to be more accurate for the unstable case but still calculates to low concentrations. Nevertheless, with accurate settings both AUSTAL2000 and CFX reach a very good agreement with the experimental data.

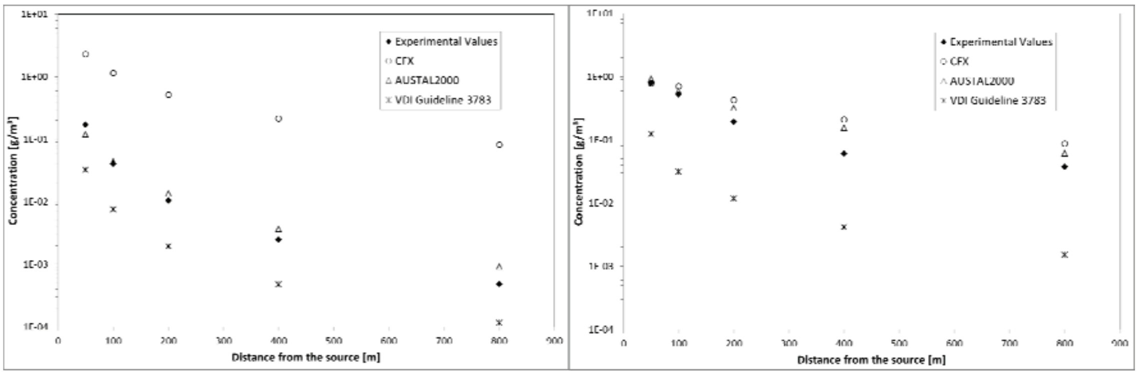

*Figure 4: Comparison of the experimental values for the Prairie Gas run Nr. 10 (left) and Nr. 36 (right) with the results of CFX, VDI Guideline 3783 and AUSTAL2000*

## 5. Conclusions

The comparison of experimental values with different gas dispersion models showed that CFD (here CFX) is able to reach good agreement with the data for very different boundary conditions and experimental setups. Specialised models like the BLM or AUSTAL2000 can achieve the same with much less effort in time, hardware and knowledge. Although under-predictive for some cases, the VDI Guideline 3783 is not only a standard tool in hazard assessment but also the only one besides CFX that is designed for heavy gas dispersion calculations. The main advantage of CFD is that it is universally applicable, as opposed to the specialised models which have a narrow scope of application. For hazard assessment purposes such as land use planning, the standard models are suitable because they give satisfactory results where CFD requires more detailed information on boundary conditions which often is not available. In case such information is available and detailed 3D information is needed, e.g. the influence on the dispersion of a new building in a plant, CFD is certainly the best choice.

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