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Comparing tools of varying complexity for calculating the gas dispersion

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ABSTRACT

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.

Keywords: Gas dispersion; Modeling; CFD; Hazard assessment; Gauss; Lagrange

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. 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 (Labovsky and Jelemenský, 2011; Luketa-Hanlin et al., 2007; Kisa and Jelemenský, 2009; Rigas and Sklavounos, 2006; Habib et al., 2013). 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 and 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 nor to account for specific boundary conditions or obstacles 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 and Janicke, 2003) and a BLM (Habib, 2011) are compared with simulations with ANSYS CFX v14.0. The aim is to point out the different capabilities and accuracies of the investigated models and to decide which level of complexity is required for hazard assessment purposes. Especially differences in the ability of resolving the near field and the theoretical ability of taking obstacles into account will influence the far field dispersion.

In order to give an estimation of the quality of each of the different approaches, open air gas dispersion experiments

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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 m were used for comparison and validation of the applied models.

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 Parts 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 center 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 100–10,000 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 and 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 and Matsugu, Sutton and Pasquill) 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 (Launder and Spalding, 1974) was used, on the one hand because, apart from its relative simplicity, it has proven to achieve good agreement with experimental results (Kisa and Jelemenský, 2009; Scargiali et al., 2005; Rigas and Sklavounos, 2006) 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). Labovsky and Jelemenský (2011) and Richards and Hoxey (1993) 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 the boundary conditions with an appropriate $k-\varepsilon$ level. Although this level will vary in the simulation domain, it was ensured that the boundary flow conditions correspond to the ones determined experimentally at the measuring points. 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