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AN LES-BASED MICROSCALE AIRBORNE HAZARD MODEL

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Abstract: First responders need a more or less instant estimate of danger zones resulting from accidentally released hazardous materials in order to take immediate action, to coordinate rescue teams and to protect human population and critical infrastructure. To fulfil the need for a sufficient dispersion modelling accuracy while maintaining efficient access to reliable results in a first responders environment, systematic high resolution pre-accidental LES modelling can be combined with 'physical data reduction' in an emergency assessment tool. A typical example of such an approach adjusted to the geometry of the Hamburg inner city area will be presented.

Key words: Accidental releases, Dispersion modelling, Emergency response tool, Hamburg pilot project.

INTRODUCTION

Manufacturing, storing and transportation of flammable and toxic gases involves the risk of accidental spills of hazardous materials. Releases of major concern occur in urban or industrial environments, with the consequence that the dispersion is heavily influenced by buildings and other obstructions. Dispersion models of different complexity have been developed in the past. Although they have been reasonably successful in some cases, most of them are still limited in scope. Especially in cases where obstacle effects dominate the dispersion of the hazardous cloud, these models are either too simplistic and thus unable to cope with the geometric complexity, or they are much too slow and thus not able to provide immediate guidance for the persons in charge of the rescue operations.

Recent progress in the fields of computer hardware development, numerical mathematics and scientific computing opens up the potential for improvements. In an effort jointly carried out by the Ministry of the Interior of the Free and Hanseatic City of Hamburg, by the US Naval Research Laboratory and by the Meteorological Institute of the University of Hamburg, a new emergency management tool for the Hamburg inner city area has been developed. This tool provides, nearly instantaneously, the space-time-structure of airborne hazardous clouds. It is based on a high- resolution LES contaminant transport model (FAST3D-CT) which provides the detailed velocity and turbulence fields within the urban domain. This database is then converted to an efficient form suitable for use in a second model (CT-Analyst) which runs on a laptop and comes with an interface as is common in computer games. The system is fast because results are pre-computed for a large number of meteorological situations. In case of an accident predictions are based solely on already existing knowledge. The system is easy to handle due to its user-friendly interface. Subsequently details of the new emergency management tool for the city of Hamburg will be presented.

THE LARGE EDDY SIMULATION MODEL

The LES simulations were carried out at the Laboratories for Computational Physics and Fluid Dynamics of the US Naval Research Laboratory in Washington. Their FAST3D-CT three-dimensional flow simulation model (Boris, 2002; Cybyk, et al, 1999) is based on the scalable, low dissipation Flux-Corrected Transport (FCT) convection algorithm (Boris and Book, 1973, 1976). FCT is a high-order, monotone, positivity-preserving method for solving generalized continuity equations with source terms. The particular FCT convection algorithm in FAST3D-CT was modified by Patnaik et al (2005).

Relevant physical processes simulated in FAST3D-CT include complex building vortex shedding, flows in recirculation zones, and approximating the dynamic subgrid-scale turbulent and stochastic backscatter. The model has the potential to also incorporate stratification, solar heating, urban greenery etc., but these features have not been used here. Emphasis was laid on capturing the effects of unsteady flow on the evolving pollutant concentration distributions.

The simulation code is designed to run efficiently on shared-memory computers. Computational grids involving about 200 million cells were typically used in the presently discussed simulations. This requires about 20 GB of memory which is now tractable on advanced computers. The challenge of high-resolution grids is not so much one of computer memory but one of computer speed. More details of the physical models in FAST3D-CT are given in Patnaik et al. (2005) and omitted here for brevity.

Runs were made separately for two domain sizes (Fig. 1a); A larger domain of 16km x 12km with a resolution of 10 m, and a smaller domain of 4km x 4km with a resolution of 2.5 m. With the exception of the upper part of the domains the cells were horizontally and vertically unstreched. Fig. 1b gives an impression of the high resolution geometry. 18 wind directions were calculated. Different wind speeds was accounted for by scaling the results according to the appropriate similarity laws. The CPU time needed pro run for one wind direction and a one hour real time episode in the small domain was approximately six days.

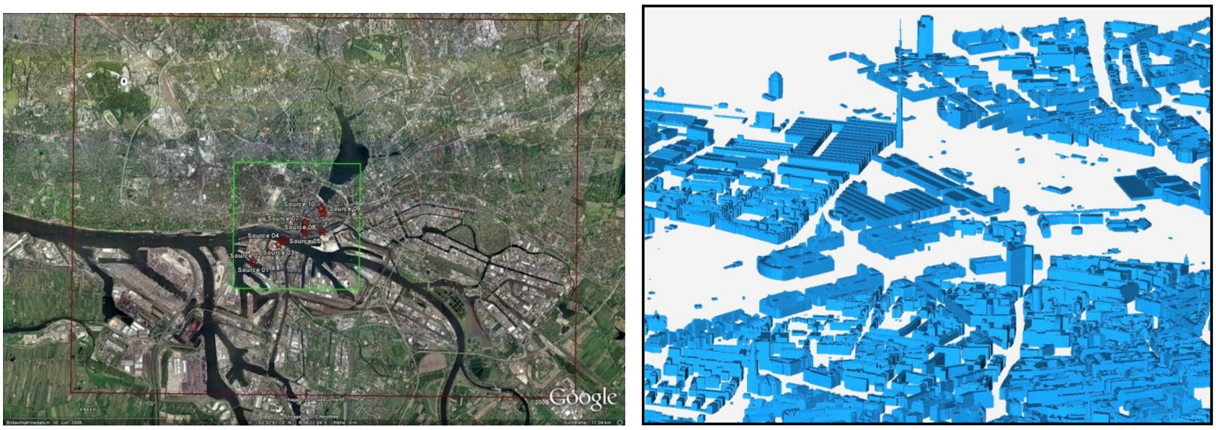

Fig. 1: (a) Top view on the 16km x 12km and 4km x 4 km domains. Lake Alster, River Elbe and the city centre are landmarks which provide orientation. (b) Sample of the 3D high-resolution geometry. The Hamburg Fair ground, the TV tower and parts of Hamburg University are easily identifiable.

For the dispersion calculations a passive, inert, gaseous tracer has been used. Passive means that the released substance drifts with the wind and spreads and dilutes due to atmospheric and obstacle generated turbulence. Buoyancy forces are neglected which, however, does not mean that the relevant substance needs to have the same density as the surrounding air. It is assumed only that the densimetric Froude number of the released cloud is well above 1. Inert means that the released gas over the period of interest neither reacts chemically nor deposits. This leads to conservative results. These are common assumptions which need not necessarily be introduced but seem to be adequate for the purpose under discussion here. With additional effort they could easily be avoided, and the FAST3D-CT code already contains the necessary physics models for these additional processes.

THE EMERGENCY MANAGEMENT TOOL

After the detailed 3D simulations for 18 wind directions are pre-computed for the coverage region, they are handed over to NRL's emergency management tool CT-Analyst® through a new data structure called Dispersion Nomografs™. CT-Analyst extends these results to all wind directions, speeds, sources, and source locations. These "nomografs" are generated well in advance, so manager using CT-Analyst in an emergency need not wait for supporting analyses (Boris, 2002).

Fig. 2a elucidates the basic method applied. The LES model provides for each grid point the local mean wind vector and the wind directional variation. Starting from a chosen source position the plume envelop can be determined by selecting at the right and left plume edge the worst case directional deviation from the mean wind vector, thereby determining the total area over which the pollutant is able to spread at all. The magnitudes of the local wind vectors determine the speed with which the cloud moves through the urban geometry. The method works likewise for instantaneous puffs and for continuous plumes, since the latter can be regarded as being made up from a series of individual puffs. Simultaneous discharges from multiple sources can be handled as well. Last but not least, the method allows placing sensors at many locations inside the domain and backtracking the signal to an up to then unknown source location.

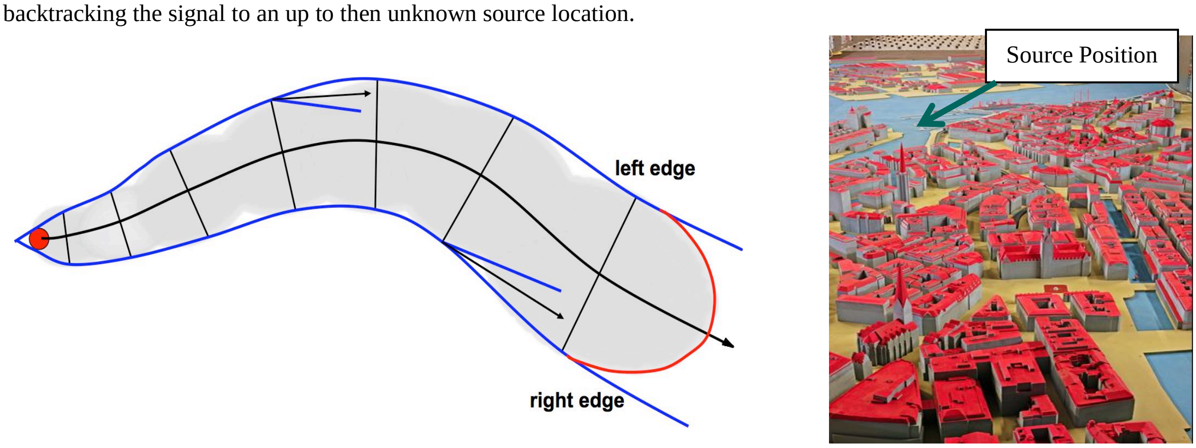

Fig. 2: (a) Top view on a plume dispersing in an environment in which obstacles effect plume shape and direction. The left and right plume edges are determined from the mean and turbulent velocity field computed by the LES model in a narrow 2.5m grid. (b) Geometrical detail of the physical model of Hamburg in the wind tunnel and indication of the source position during the field tests.

Although the immediate knowledge of the total area over which a pollutant can spread is certainly the most important information for a first responder, the second question concerns the pollutant concentrations. For these conservative estimates are provided only. Since the sources can be anywhere in the domain, the huge number of possible concentration fields are not directly calculated by the LES model. Instead of this, the plume edges in combination with a plume profile assumption are used to determine the local mean concentrations as a function of source strengths, simply by applying the mass conservation principle. Variability around the mean value is roughly estimated from mean to peak ratios determined for a few spills released at representative positions in LES model experiments. Taking into account that reasonable thresholds for short time peak concentrations are often not available, this seems to be an acceptable constraint.

VALIDATION OF THE EMERGENCY MANAGEMENT SYSTEM

In order to demonstrate the quality of the emergency management system, validation data sets have been generated in field and wind tunnel experiments. The wind tunnel experiments were carried out in the large boundary layer wind tunnel 'Wotan' of Hamburg University. This tunnel has a total length of 25 m with a test section which is 4 m wide and 2.75 m high and contains a flow establishment section of about 18 m length. The wind tunnel is equipped with an adjustable ceiling allowing 0.5 m height extension of the test section. An approach flow boundary layer matching the scale of the Hamburg model (1:350) was generated. The boundary layer properties were controlled and documented similarly as described in Schatzmann and Leitl (2011) for another wind tunnel investigation. Non-intrusive flow measurements were carried out with an optical LDA fibre probe with a focal length of 800 mm. To measure high resolution concentration time series a fast flame ionisation detector was used. Fig. 2b shows a sector of the (in full scale) 3700m long and 1400m wide physical model in the wind tunnel. Under steady-state mean flow conditions numerous instantaneous and continuous clouds were released at multiple positions and time series of the resulting velocity and concentration fields were monitored. Details of the comparison between wind tunnel and numerical model results will not be given here; they are subject of the accompanying papers by Hertwig et al. (2011) on the flow and turbulence characteristics and by Harms et al. (2011) on the properties of the dispersing pollutant. Here it is mentioned only that the LES model results very satisfyingly matched the wind tunnel data although neither side knew the results of the other side beforehand (blind testing).

Two short field campaigns were carried out in addition to the wind tunnel experiments. Such field tests are always limited in scope. As was described in more detail in Schatzmann and Leitl (2011), it is nearly impossible gaining reliable test data for complex CFD models in such experiments. The atmosphere is intrinsically time dependent and never steady state. The commonly assumed 15 min or 30 min quasi-steady episodes exhibit a large inherent variability. Data obtained over such short periods of time are not representative for the assumed mean wind velocity and direction. And even worse, in urban canopy layers it occurs to be nearly impossible to determine a position at which a representative wind vector could be measured. Nevertheless comparisons with field data are vital for building confidence in the quality of numerical and physical model predictions; whenever possible they should be carried out.

To perform field measurements in a vibrant metropolitan area is, however, hardly feasible. Permission for carrying out dispersion experiments was granted only for a few early morning hours at 2 weekends. With strong support by fire-fighters and police of the city of Hamburg small amounts of SF_6 were released upwind from the city centre from a boat positioned at river Elbe. In cooperation with scientists from the Forschungszentrum Jülich about 20 automated bag samplers were distributed over the inner city area (Fig. 3a). The probes were subsequently analyzed by using gas chromatography.

Fig 3: (a) Measurement positions during the field experiments and (b) picture of an automated bag sampler rig in front of the Hamburg town hall.

Early morning observations are always somewhat of a problem. During the first observational period at April 16, 2011, there was high pressure over Hamburg with clear skies and large radiative cooling of the surface. Such weather situations are subject to stratification and inversion layers, and this was indeed the case as the measurements at the Hamburg TV-Mast approximately 10 km apart from the site clearly indicate. As becomes evident from Fig 4a, there was a strong inversion above the 110 m measurement platform although the wind speed at higher altitudes was quite strong (Fig 4b). As smoke experiments carried out at the end of the intensive operation period evidenced, there were even more inversions near the ground. None of the altogether 8 ultra-sonic-anemometers which were operated simultaneously at different locations around the test site provided a wind speed and direction which matched the movement of the smoke cloud.

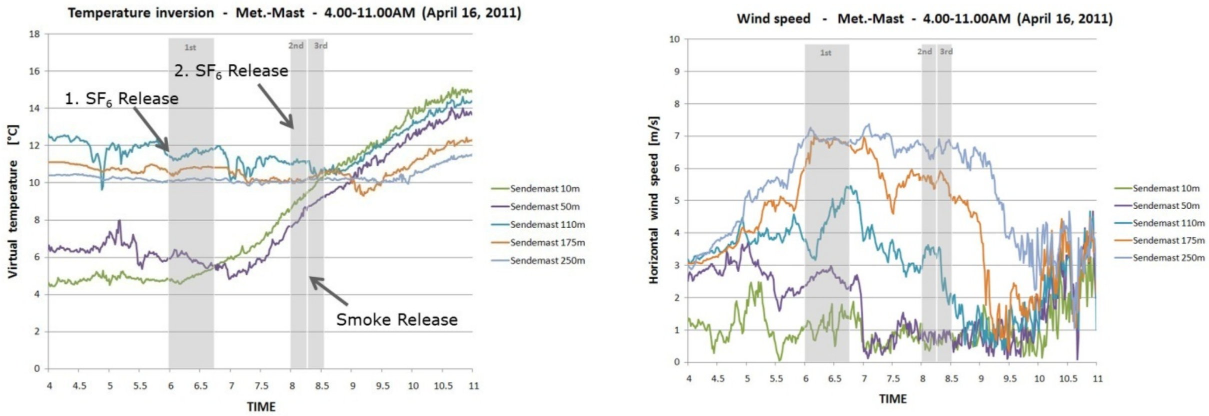

Fig. 4: Virtual temperatures (a) and wind velocities (b) measured during the first experimental period at 5 different height levels at a TV mast located about 10 km apart from the test site at the eastern edge of Hamburg.

With the second field experiment we waited until a really stormy weekend with winds from the favoured directional sector arrived. Although highly fluctuating with time, wind speed and direction were much more uniform compared to the first campaign (Fig 5b). This finding was fully corroborated by the measurements performed at different height levels at the Hamburg TV mast. In contrast to Fig. 4, in the second phase the boundary layer was well mixed. The wind directions in the lowest 250 m above ground were always around 220°, independent of height and time, and the velocity profile only slightly increased with height.

The automated samplers were spread over an area much wider than the expected cloud width in order to identify not only polluted but unpolluted areas as well. Although the time resolution of the field data is insufficient for the purpose of LES model validation, the overall agreement is generally good. A comparison of measured and predicted concentrations is under preparation. However, since the bag samplers average over an intermittently fluctuating contaminant supply rate, large variability bars would have to be added to the measurements. The magnitude of these bars remains unknown since short-time experiments do not provide the information necessary for statistical analyses (see Schatzmann and Leitl, 2011). Further comparisons between field data, wind tunnel data and numerical results are under preparation. They also comprise FTIR measurements which were carried out by the Technical University of Hamburg-Harburg in combination with Bruker Sigma.

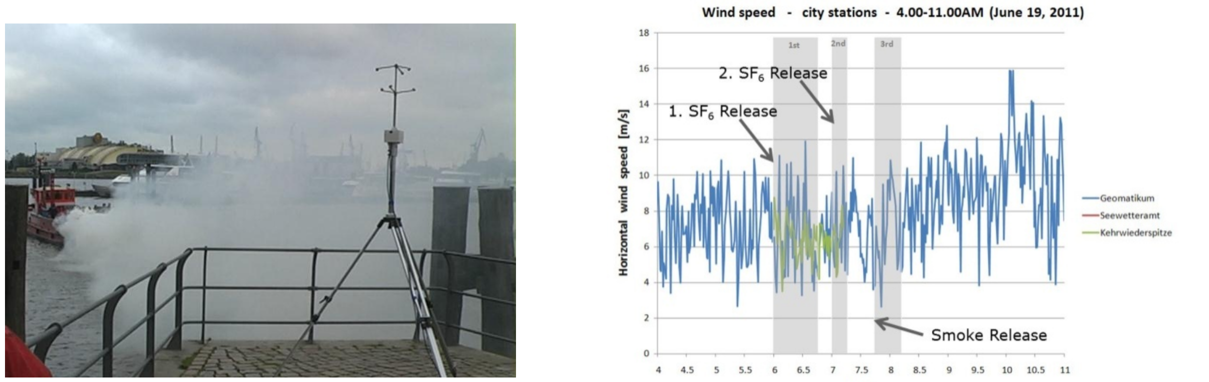

Fig. 5: Second campaign at June 19, 2011: (a) Picture from the highly meandering smoke plume and from the ultra sonic anemometer located at 'Kehrwiederspitze'. (b) Wind velocity versus time trace measured simultaneously at 2 different stations during the intensive operation period on June 19, 2011.

CONCLUSIONS

Accidental or deliberate releases of harmful agents in urban areas can produce a tremendous challenge to emergency response staff even if the amount of the released substance is small and the scale of the thread limited. This is partly caused by the fact that the dispersion process in complex geometries is driven by complex wind flows and turbulent diffusion. From a strict physical point of view, the source sizes, release rates or (mostly short time) durations of release events often restrict the use of tools which are based on mean flow and dispersion modelling because in the atmosphere the assumed mean conditions do not exist for relevant time periods less than many hours of constant weather.

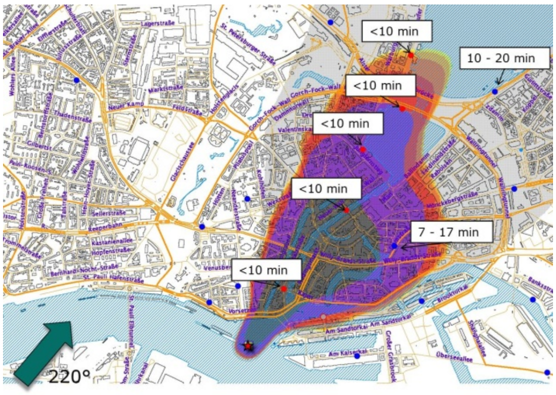

Fig. 6: Second campaign at June 19, 2011. Bag sampler positions are shown with red dots polluted and blue dots unpolluted. The bag-samplers operated time-staggered with suction intervals of 10 min. Comparison of cloud contours predicted by the emergency management tool with measured results (a) 5 min after the release and (b) 10 min after the release.

Therefore it is necessary to move forward to advanced modelling technics which have the potential to deal with the unsteady behaviour of local scale dispersion in complex geometries in a more consistent way. As was shown, technical progress has advanced and a new generation of CFD models is ready to be applied in the context of dispersion predictions for hazardous clouds resulting from accidental releases in urban or industrial environments. Although these models of LES type are very demanding with respect to computational hardware and time resources, they can be applied before an emergency occurs. In combination with an intelligent tool which excerpts the relevant information from the simulated CFD results first responders receive immediate decision making assistance.

A prototype of such an emergency management system adjusted to the geometry of the city of Hamburg has been developed and validated with data from appropriate wind tunnel and field experiments. The results obtained so far are promising. At the end of 2011 the new emergency management system will be handed over to the city authorities and tested under realistic operating conditions.

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