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MODITIC

modelling the dispersion of toxic industrial chemicals in urban environments

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Summary

The main objective of the MODITIC (Modelling the disperison of toxic industrial chemicals in urban environments) project is to enhance our fundamental understanding of the physical processes and the associated challenges regarding modelling the dispersion of non-neutral gasses in built-up environments. The project goal is to lay the ground for future improvements of dispersion models used in emergency situations by military personnel as well as civilian emergency services, thereby contributing to the improvement of emergency preparedness and response.

To achieve these goals, atmospheric wind tunnel experiments have been systematically applied and novel experimental data sets for a number of carefully chosen dispersion scenarios have been provided. The same set of configurations has also been subject to computational modelling efforts using both advanced Computational Fluid Dynamics (CFD) and simpler Gaussian models. Experimental data for the release of toxic chemicals from pressurized vessels have also been made available to the project in order to provide realistic source characterisations in the case of an event. Accompanying computations using the conditions of the release experiments have been conducted in order to validate computational models and to identify their weaknesses.

The project has generated a large database comprising experimental and numerical results for release and dispersion of neutral and dense gasses in configurations ranging from simple to complex geometries. This database will be a valuable addition to the body of reference data needed to advance the fundamental understanding of dispersion in urban environments and its modelling. The database may be used for development, improvement and validation of dispersion models for hazardous materials in urban environments.

The scientific methodology adopted in MODITIC, where numerical simulations have been conducted together with wind tunnel experiments and field trials, have proven to be very successful. This approach is recommended to be used also in future projects, including the follow-up project MODISAFE (CRN modelling of sources and agent fate).

Sammendrag

Hovedmålet med MODITIC-prosjektet (Modelling the disperison of toxic industrial chemicals in urban environments) er å forbedre vår grunnleggende forståelse av spredning av ikke-nøytrale gasser i bebygde miljøer. Prosjektet har som mål å legge til rette for fremtidige forbedringer av spredningsmodeller som brukes i krisesituasjoner av militært personell og sivile nødetater, og dermed gi bedre beredskap og respons.

Atmosfæriske vindtunneleksperimenter har blitt systematisk gjennomført, og nye eksperimentelle datasett for en rekke nøye utvalgte spredningscenarier er blitt produsert. De samme konfigurasjonene er også blitt modellert ved bruk av både avansert Computational Fluid Dynamics (CFD) og enklere gaussiske modeller. Prosjektet har også fått tillgang på eksperimentelle data for utslipp av giftige kjemikalier fra trykksatte tanker som har blitt brukt for å gi realistiske kildekarakteristikker ved denne type hendelser. Beregninger av disse utslippseksperimentene har blitt utført for å validere beregningsmodellene.

Prosjektet har generert en stor database med eksperimentelle og numeriske resultater for spredning av nøytrale og tunge gasser i konfigurasjoner som spenner fra enkle til komplekse geometrier. Denne databasen vil bli gjort tilgjengelig. Den gir referansedata som er nødvendige for å forbedre den grunnleggende forståelsen av spredning av gasser i urbane omgivelser og for modellering av spredningen. Databasen kan anvendes for utvikling, forbedring og validering av spredningsmodeller for farlige kjemikalier i bymiljø.

Den vitenskapelige metode som er brukt i MODITIC, der numeriske simuleringer er utført sammen med vindtunnelforsøk og feltforsøk , har vist seg å være svært vellykket. Denne tilnærmingen anbefales også i fremtidige prosjekter, deriblant oppfølgingsprosjektet MODISAFE (CRN modelling of sources and agent fate).

Contents

Preface

This work is part of the European Defence Agency (EDA) project B-1097-ESM4-GP “Modelling the dispersion of toxic industrial chemicals in urban environments” (MODITIC). The scientific objective of this project is the systematic study of the release and transport of neutral and non-neutral chemicals in complex urban environments, to enhance understanding of the dominating physical processes involved, and to support improvements in modelling techniques. The participating organisations are:

- Direction Générale de l’Armement (DGA), DGA CBRN Defence, France
- Institut National de l’Environnement Industriel et des Risques (INERIS), France
- Norwegian Defence Research Establishment (FFI), Norway
- Swedish Defence Research Agency (FOI), Sweden
- University of Surrey (UoS), United Kingdom

FFI is the lead organisation. The project was initiated September 1, 2012, with duration of three-and-a-half years. The project is funded by the Norwegian Ministry of Defence, the Swedish Ministry of Defence, the French Ministry of Defence, and the French Ministry of Ecology, Sustainability and Energy.

1 Introduction

Toxic industrial chemicals (TICs) are used in most countries, and are produced, transported and stored in relatively large quantities. The possible consequences of accidental or intentional release of such compounds are of concern both to military and civilian authorities. Possible hazardous releases may occur due to accidents, sabotage, or terrorist actions at industrial complexes or during transport of hazardous materials. Military and civilian authorities need fast and reliable information about the type of hazardous agent, location(s), and rate(s) of release, total amount of release, airborne transport, and dispersion predictions of concentration, deposition, and dosage levels, and consequence assessments in order to plan and take appropriate actions. There is a continuous need to update, refine, and display the overall picture of the emergency situation, based on sensor information, human observations, and other possible and available information sources. Consequence assessment of selected scenarios using dispersion modelling is an important tool for emergency response and consequence management planning, training, and exercises.

Several important TICs are buoyant, i.e. heavier-than-air gasses such as chlorine and sulphur dioxide, or lighter-than-air gasses, such as ammonia. Dispersion modelling of buoyant TIC in complex urban environments poses severe challenges. In addition to the complex topography in such environments, the density differences between the TIC and the ambient air may severely alter dispersion processes. Hence, under appropriate conditions, a lighter-than-air emission may rise from the ground whereas a heavier-than-air emission may remain near the surface. The latter will possibly create strong stable density gradients that greatly reduce air entrainment and thus the mixing process. For instance, mixing can be effectively eliminated in regions of the urban terrain with very low wind speeds and toxic chemicals may remain for long period of times.

Current prediction methods are associated with very large uncertainties. The lack of high-quality measurements adversely affects the much needed development of improved numerical models and the understanding of the uncertainty in their performance. These uncertainties manifest themselves in all dispersion models, either when compared with each other or with experiments, and also in the interpretation of model output in an operational context.

The main objective of the European Defence Agency (EDA) Project "Modelling the dispersion of toxic industrial chemicals in urban environments" (MODITIC) is to enhance our fundamental understanding of the physical processes and the associated challenges regarding modelling the dispersion of heavier-than-air gasses in built-up environments. The project goal is to lay the ground for future improvements of dispersion models used in emergency situations by military personnel as well as civilian emergency services, thereby improving emergency preparedness and response.

The project work encompasses atmospheric wind tunnel experiments on neutral and dense gas dispersion for a selection of geometries with increasing complexity. Selected geometries were subject to computational modelling efforts using both advanced Computational Fluid Dynamics (CFD) and simpler Gaussian models to investigate performance of various numerical methods. In addition, special data sets were compiled to examine inverse modelling capabilities. The project also made use of available experimental data for outdoor and indoor ammonia releases from pressurized vessels in order to test modelling strategies to realistically characterise the release.

2 Agent characterization and source modelling

Toxic industrial chemicals are often stored under pressure in a liquid state in large tanks or vessels. If there are tank failures and/or leakages in an urban area, part of the released liquid forms a jet that undergoes a flashing process and parts spills directly onto the ground (rainout). Rainout to the ground may also appear when the jet impinges a wall. The resulting rainout pools constitute secondary vapor sources. The jet is thus a complicated mixture of liquid aerosols, vapor, and entrained air.

The MODITIC project investigated the capability of CFD models to handle dense multiphase jets impinging on obstacles have been investigated. This includes modelling the flashing, expansion, evaporation, and rainout processes. Experimental data for the release of toxic chemicals from pressurized vessels [1] have been made available to the project in order to provide realistic source characterizations in the case of such an event. Accompanying computations using the conditions of the release experiments have been conducted in order to evaluate computational models. Experimental data from large scale ammonia releases [1] have also been made available and used for comparison with simulation results using Gaussian models.

None of the institutes involved in MODITIC have a CFD capability which can fully model all the physical processes associated with a two-phase release of ammonia. Interaction with an obstacle close to the release adds further complexity to the behaviour of the multi-phase turbulent jet. The impact on an obstacle and the subsequent drainage to the ground of a liquid fraction remains to be studied. On the other hand, it is currently possible to integrate part of the source term as an empirical term in complex CFD models, by specifying the form and content of liquid and gas mass fractions, discharge rates and energy content at the end of the expansion phase, and to compute the following dispersion and air entrainment. Finally, in order to handle a CFD source term such as a dense gas released from a ruptured vessel in an urban area, a decoupled approach is recommended that separates the rapid phenomena (flashing and expansion) that need empirical descriptions, and slow phenomena (gas dispersion and entrainment) that can be computed using CFD [2].

3 Atmospheric wind tunnel experiments

Atmospheric wind tunnel experiments have been systematically applied and detailed experimental data sets for a number of carefully chosen dispersion scenarios have been provided. Project planning identified six categories of increasing complexity, the aim being to ensure gradual progress in complexity that, in turn, would lead to progress in understanding and capability for both forward and inverse modelling, namely:

1. Flat surface
2. Two-dimensional hill
3. Two-dimensional back-step
4. Simple array of obstacles
5. Complex array of obstacles
6. An urban area (central Paris, see Figure 3.1).

Each of these categories was further sub-divided by studying different wind directions, emission conditions (continuous and finite duration), and data requirements. The extensive series of experiments was conducted in the EnFlo 'meteorological' wind tunnel at the University of Surrey (UK) to generate data both to evaluate dispersion models and to aid understanding of underlying physical processes. Two component laser-Doppler anemometer (LDA) and fast flame ionisation detector (FFID) instrumentation were used to measure the flow and concentration fields in categories 2. – 6. (suitable data were already available for category 1.) for a range of source locations and emission conditions (non-buoyant and dense gas) in a simulated neutrally stable atmospheric boundary layer. The overall strategy was to use operating conditions that were consistent with good quality flow in the wind tunnel but produced significant dense gas effects in the carbon dioxide plumes; e.g. as exemplified by upwind and enhanced lateral spread. The data are contained in a collection of text and Excel files with supporting meta-data, comprising in total a very extensive and detailed data-base of dispersion in complex environments. Included in the data-base is a collection of long, simultaneous data series from four FFIDs that can be used in investigating inverse modelling capabilities. More information about the experimental work can be found in [3].

Figure 3.1 *The Paris model installed in the meteorological wind tunnel.*

4 CFD modelling

High fidelity computational fluid dynamic methodologies based on both Reynolds Averaged Navier Stokes (RANS) and Large Eddy Simulation (LES) modelling have been applied In the MODITIC project.

RANS models have a number of applications where they produce good results, but the models are not general and cannot be used for all types of problems. Therefore it is important to evaluate different types of RANS models for a range of scenarios to make the range of usefulness clear. Here, most scenarios were evaluated using the linear $k - \varepsilon$ model and the $k - \varepsilon$ MMK-model [4].

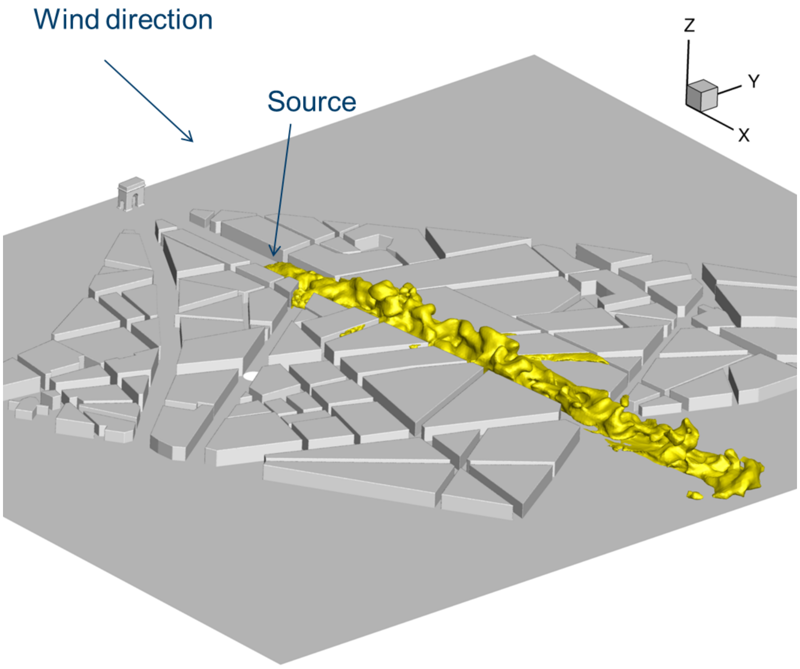
The results show that both models capture the main features of the flow: turbulence levels and flow directions are mainly in line with the findings from the experiments ([5]). Comparison of predictions for the neutral releases shows that both models can capture the turbulent transport. However, the buoyancy effects in heavy gas releases are only partially captured.

A possible improvement would consist in using low-Reynolds models, such as the $k - \omega$ SST model [6], and more refined meshes in stratified regions to better capture the boundary layer and the dense plume edge gradients. It would be also worth investigating algebraic flux models to better capture anisotropic turbulent viscosities, and local Richardson number dependant damping factors in isotropic turbulent viscosities.

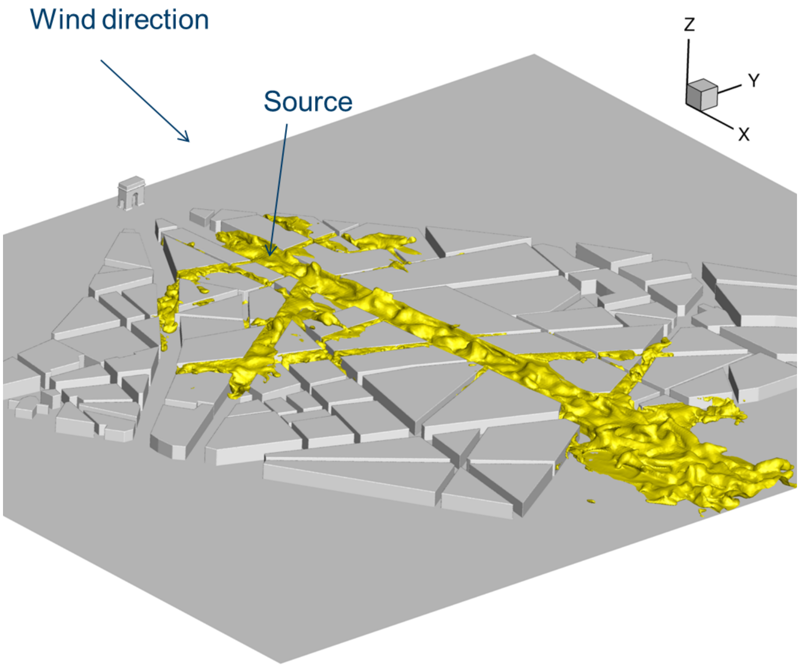
Large Eddy Simulations represent the current state-of-the-art method in advanced dispersion and transport modelling of gasses and aerosols. In this project, the LES methodology has been applied to model dispersion of neutrally buoyant and dense gas in the geometries tested in the wind tunnel ([7]). Different methods of providing inflow conditions have been utilized as well as different ways to describe the dense gas.

The changes the dense gas exerts on the wind field are validated against experimental results with good agreement, as are the concentration fields, Reynold stresses, and turbulent mass fluxes. Interesting characteristics of the dense gas dispersion are the upstream spread and the wider and shallower plume. Obstacles affect the dense gas to a higher degree compared to a neutral release because the dense gas remains closer to the ground, within the influence of individual buildings and street networks. Figure 4.1 shows the neutral and dense gas plume developed after release from a source located in Champs-Élysées in Paris. Here, the difference in dispersion pattern between dense and neutral gas is easily seen, with dense gas being transported upstream of the source, keeping closer to the ground, and dispersing more laterally.

In the MODITIC project, it has been shown that the LES methodology used is suitable to predict both dense and neutrally buoyant releases of gas within an urban environment. However, in order to assure satisfactory results, special care needs to be taken concerning the inflow conditions with regard to the spatial and temporal resolution of the incoming boundary layer.



(a) Neutral gas



(b) Dense gas

Figure 4.1 *Gas plume of neutral and dense gas released from a source placed in Champs-Élysées in Paris.*

5 Operational urban dispersion modelling

The MODITIC project has used four different operational models for different geometries spanning from open field dispersion to the complex geometry of central Paris. These are ARGOS, PUMA, Gaussian-puffs-QUIC, and Parallel Micro Swift Spray (PMSS) (see [8] for description of the models). Referring to COST action ES1006 ([9], [10]) on the use of atmospheric dispersion models in emergency response tools, a number of statements can be confirmed ([8]):

- The different types of operational tools require different skills and expertise levels. Execution times for the simulations vary from minutes to hours. The most time consuming and demanding part is to setup the models and to couple them to meteorology and source term descriptions.
- The choice of output to give to decision makers is not straightforward; e.g. it might be risk zones corresponding to concentrations, confidence intervals or percentiles within a specified limit.
- The models are usually conservative and overestimate the concentration levels close to the source (e.g. as demonstrated by the use of ARGOS for the Paris scenario).

5.1 Dense gas effects

Predictions from QUIC software ([11]) seem to compare well with experimental data ([1]) using the included dense gas sub-model. PUMA also gives promising results. The latest developments of PUMA have been tested within the scope of this project, dealing with dense puff interaction in a semi-linearized way to keep the response fast enough. The ARGOS ([12]) heavy puff model works well compared to experimental ammonia release [1], but cannot handle obstacles at the same time.

5.2 Obastacles

The ARGOS Urban Dispersion Model (URD) necessitates scaling up small obstacles (e.g. the INERIS case with wall) and is more suited to a densely built urban-like area (e.g. the Paris case, with a source surrounded by buildings). A “real” case with hydrogen cyanide was considered by scaling up the wind tunnel flow conditions. The URD model can handle passive gas only, so no dense gas–obstacle interaction could be tested and validated. In the Paris case, a tendency to overestimate by a factor of three to five close to the source, and underestimate by the same factor in the far field was observed and explanations were proposed. PUMA is not able to include obstacles and is therefore not suitable for complex geometry cases. The PMSS model ([13]) was tested against the “complex array of obstacles” and Paris cases ([3]) for passive gas only, and behaved reasonably well. Overestimations of concentrations behind buildings and underestimations in main streets were usually observed. The QUIC software is currently able to handle both obstacles and dense gas.

Finally, it should be emphasised that these methods are not push-button tools and require user expert skills. Their advantage compared to CFD is a cheap computational cost, but they still need relatively large set-up times compared to the run-time.

6 Inverse modelling

Linear inverse dispersion modelling, in particular from a single point source, is a maturing field where least square optimisation methods as well as Bayesian approaches have been adapted to solve the problem. In many studies, however, the setting is both oversimplified (flat terrain, Gaussian plume dispersion models) and the detector data generated synthetically. In MODITIC we have brought linear inverse modelling to an urban environment (there are up to 14 buildings in the town studied) and we use detector signals from MODITIC wind tunnel experiments of the same configuration. Two different methods, renormalisation [14] and a Bayesian framework (see e.g. [15]), have been used to solve the resulting inverse problem. Both methods rely on having adjoint functions for computational efficiency. In this case the adjoint fields are RANS CFD-fields. Preliminary studies, as well as the literature, indicate that for flat terrain the location of the reconstructed source will have a good accuracy in the cross wind direction while the uncertainty is much larger in the wind direction. As a knock-on effect the release rate will also reflect the corresponding uncertainty: a source located further away will have to release more mass per time unit to render the detection readings in the correct range. Comparison of the two inverse solving methods for the built-up environment for neutral releases show that the results keep within expectations: since there is no change in the prevailing wind direction there is little uncertainty in the source location in the cross wind direction, but significantly more in the direction along the wind direction.

Hence, it is concluded that the inverse methods work acceptably well in the urban setting with neutral releases: the primary operational challenge lies in generating adjoint plumes capturing the dispersion process [16]. An even greater challenge is the treatment of dense gas emissions, because of the non-linear relationship between dispersion behaviour and emission strength, and it remains unclear how reliable and operationally feasibly inverse modelling capabilities for dense gas releases should be formulated.

7 Conclusion

The scientific methodology adopted in MODITIC, comprising of numerical simulation together with wind tunnel and large scale experiments, has proven to be an extremely successful approach and will be used in upcoming projects.

The project has generated a large database comprising experimental and numerical results for release and dispersion of neutral and dense gasses in complex geometries. The experimental data cover a range of realistic scenarios of increasing complexity, from a flat, open surface to the centre of Paris. This database will be a valuable addition to the body of reference data needed to advance the fundamental understanding of dispersion in urban environments and its modelling. The database may be used for development, improvement and validation of dispersion models for hazardous materials in urban environments.

In the project, gap of knowledge was identified for, among others, source characterizations. A follow-up project called MODISAFE will work on improving the knowledge and representation of source characteristics as well as loss processes, such as deposition and absorption. The aim of the project is to develop or improve models describing these and other phenomenas inadequately dealt with in current models, inter alia, by using the knowledge gained from MODITIC.

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About FFI

The Norwegian Defence Research Establishment (FFI) was founded 11th of April 1946. It is organised as an administrative agency subordinate to the Ministry of Defence.

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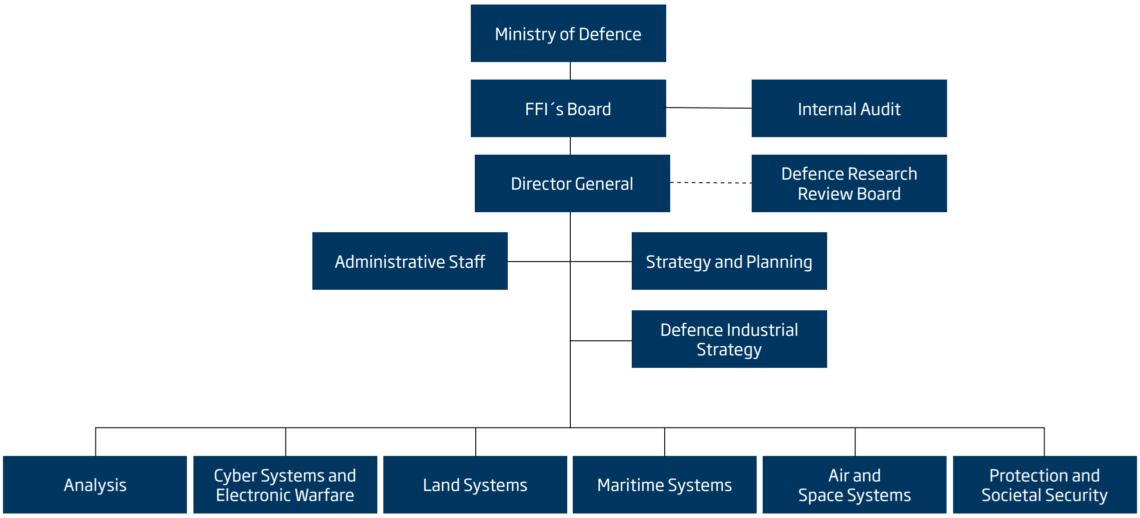

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