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MODITIC - MODELLING THE DISPERSION OF TOXIC INDUSTRIAL CHEMICALS IN URBAN ENVIRONMENTS

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Abstract: The main objective of the MODITIC project is to enhance our fundamental understanding of 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 improving emergency preparedness and response. 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 in order to provide realistic source characterisations in the case of an event have also been made available to the project. Accompanying computations using the conditions of the release experiments has been conducted in order to validate computational models. 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.

Key words: *MODITIC, dense gas dispersion, urban environments, wind tunnel experiments, Computational Fluid Dynamics, RANS, Large Eddy Simulations, linear inverse modelling*

INTRODUCTION

Toxic industrial chemicals 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. 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 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 characteristics.

The MODITIC project results is summarised below under six headings corresponding to the various activities. Further details are available in the accompanying papers.

ATMOSPHERIC WIND TUNNEL EXPERIMENTS

Atmospheric wind tunnel experiments at the University of Surrey (Robins *et al*., 2016) 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. A flat surface
2. A two-dimensional hill
3. A two-dimensional back-step
4. A simple array of obstacles
5. A complex array of obstacles
6. An urban area (central Paris).

Each of these categories was further sub-divided by wind direction, emission conditions (continuous and finite duration), and data requirements. In support of the overall project aims, an 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 to 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.

SOURCE TERM EXPERIMENTS AND COMPUTATIONS

Large scale ammonia release experimental data have been made available and used for comparison with simulation results using 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 such an event. Accompanying computations using the conditions of the release experiments have been conducted in order to validate computational models.

Toxic industrial chemicals are often stored as pressurized liquefied gas. A vessel failure or rupture induces a violent two-phase release of liquid and gas (thermodynamic flash), that current CFD models used by the MODITIC project partners are not able to deal with in all its complexity. Interaction with an obstacle close to the release adds further complexity of 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, and rates, energetic contents 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 between rapid phenomena (flashing and expansion) that need empirical descriptions, and slow phenomena (gas dispersion and entrainment) that can be computed using CFD.

OPERATIONAL MODELS

The MODITIC project has used four operational models for different geometries spanning from open field dispersion to the complex geometry of central Paris. The four models are ARGOS, PUMA Gaussian-puffs-QUIC, PMSS: Lagrangian (see Björnham *et al*., 2016 for description of the models). Referring to COST action ES1006 (COST ES1006 (1), COST ES1006 (2)) on the use of atmospheric dispersion models (ADM) in emergency response tools (ERT), we confirm a number of statements (Björnham *et al*., 2016):

- The different types of operational tools require different skill or expertise levels. The execution time for the simulations varies from minutes to hours. The most time consuming and demanding part is the setup of the models and to couple them to meteorology and source term descriptions.
- The type of response to give to decision makers is not straightforward: shall we give risk zones corresponding to concentrations, confidence intervals or percentiles to be in such limits.
- These models are usually conservative, and overestimate the concentration levels close to the source (as demonstrated by the use of ARGOS for the Paris scenario).

Regarding dense gas in operational tools, QUIC software (Los Alamos National Laboratory, 2016) seems to compare well with INERIS data (Gentilhomme, 2013) using the included dense gas sub-model, and PUMA also gives promising results. These last developments on 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. ARGOS (PDC-ARGOS, 2016) heavy puff model works well on INERIS ammonia release, but cannot handle obstacles at the same time.

Regarding obstacles, ARGOS Urban Dispersion Model (URD) necessitates scaling up small obstacles (INERIS case with wall) and is more suited to a densely built urban-like area (Paris case, with source surrounded by buildings). The URD model can handle passive gas only, so no dense gas-obstacle interaction could be tested and validated. On the Paris case, tendency to overestimate by a factor of three to five close to the source, and underestimate by such in 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 model Parallel Micro Swift Spray (PMSS) (ARIA VIEW, 2016) was tested against the "complex array of obstacles" and Paris cases (Robins *et al.*, 2016) 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. In the study with ARGOS, a "real" case with hydrogen cyanide was considered by scaling up the wind tunnel flow conditions.

Finally, these tools are not push-button tools and require expert skills. The advantage against CFD is their cheap computing cost, but they still need relatively large set-up times compared to the run-time.

RANS SIMULATIONS

Reynolds-averaged Navier-Stokes (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. Thus it is important to evaluate different types of RANS-models for a range of scenarios to make clear what the range of usefulness is. 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 experiment (Burkhart and Burman, 2016). The comparison of the neutral release shows for both models that they can capture the turbulent transport. The heavy gas release though, indicates that the buoyant effects are only partially captured. A possible improvement would consist in using low-Reynolds models such as $k\omega$–sst and more refined meshes in stratified regions to better capture the boundary layer and the dense plume edge gradients. It would be also worth investigate algebraic flux models to better capture anisotropic turbulent viscosity, or damping factors in isotropic turbulent viscosity as a function of local Richardson number.

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 (Issartel *et al*., 2012) and a Bayesian framework (see e.g. (Stuart, 2010)), 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 be associated with 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.

We therefore conclude that the inverse methods work acceptably well in the urban setting with neutral releases: the challenge lies in generating adjoint plumes capturing the dispersion process (Brännström *et al.*, 2016). An even greater challenge is the treatment of dense gas emissions.

LARGE EDDY SIMULATIONS

Large Eddy Simulations (LES) represent the current state-of-the-art method in applied turbulence research. 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 (Wingstedt *et al*., 2016). Different methods of providing inflow conditions have been utilized as well as descriptions of the dense gas. The changes the dense gas exerts on the average wind field are validated against experimental results with good agreement as well as 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 within the street network.

The conclusion is that the LES methodology used within the MODITIC project is suitable to predict both dense and neutrally buoyant releases of gas within an urban environment. One of the major findings is that care should be taken concerning the inflow conditions with regard to the spatial and temporal resolution of the incoming boundary layer.

MAIN RESULTS AND CONCLUSIONS

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.

FUTURE WORK

One of the primary scientific objectives of MODITIC has been to study the interactions between a dense gas and the wind field in the vicinity of the source. These are very complex dynamical interactions that pose particular challenges for a modeller. A similar, and an oftentimes occurring situation, is the dispersion of gasses and aerosols in a stably stratified atmospheric background. One obvious follow-on study to MODITIC would be to benefit from the experiences and lessons learned in the application of a wide range of models with different complexity and repeat the work in stable boundary layers. Similar work could also be carried out in unstable boundary layers, including the study of bouyuant sources (e.g. fires). Topics that deserve further and deeper study include the relation between upwind and lateral spread near the source and the emission properties and the adaptation of street network dispersion models to dense gas emissions.

The project partners will continue analysing and exploiting the MODITIC data to fill knowledge gaps related to dense gas dispersion. This includes the development of an inverse model for dense gas dispersion in urban environments. A systematic study of the dynamic interaction between a dense gas cloud and the wind field in the vicinity of the source in a massively separated boundary layer will be investigated using MODITIC experimental data and LES. The data from both experiments and LES computations will also be put to good use in the development of improved models based on the RANS method. The practical experiences with dense gas releases in a wind tunnel environment will be beneficial in future studies.

The project partners are planning a new European Defence Agency (EDA) project entitled "CR MODellIng of Sources and Agent FatE" (MODISAFE) aimed to start 1 January 2017, which builds on and supplements MODITIC. Processes such as evaporation, deposition fractions on environmental surfaces such as the ground, buildings and vegetation, as well as suspension and re-suspension of particles greatly influence the resulting hazardous concentrations of various threat agents, thus should be properly dealt with in modelling and simulation approaches and hazard prediction tools. The project will perform both experimental and numerical work and contribute to improved scientific knowledge and to advance the state-of-the-art operational models used for emergency response.

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