17th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 May 2016, Budapest, Hungary

MODITIC OPERATIONAL MODELS

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Abstract: Events including toxic substances can be dangerous and difficult for first responders to handle since there is often limited time for decisions regarding evacuation of nearby regions. There are many quick operational models that simulate atmospheric dispersion and thereby provide guidelines for which risk area to expect. A few different models are evaluated in this work against real scale and wind tunnel experiments with the main emphasis on dense gas. The models have different merits and shortcomings with regards to their ability to handle dense gases and complex geometries which are briefly covered here.

Keywords: *Atmospheric dispersion, QUIC, PUMA, ARGOS, Lagrangian model.*

INTRODUCTION

Unexpected events involving hazardous substances are of growing concern in today´s societies. In the case of an outdoor release, the area of impact is by far the largest if the released substance is in gaseous form. The ambient advection and turbulence of the air will then lead to a dispersion process causing a spread and subsequent dilution of the concentration. Many chemicals are stored as liquefied gas for practical reasons. The rapid decrease of pressure after a sudden release in combination with a limited infusion of heat leads to a dense gas dispersion. This means that the released substance is in gaseous form with high density and will therefore spread close to the ground, which strongly reduces the vertical dilution process resulting in an increased area of potentially dangerous concentration levels. Dense gas modelling has been the main target for the EDA project MODITIC which has treated many aspects of the problem. The project has included large scale field experiments and downscaled wind tunnel experiments. These results have then been used to benchmark different models that simulated the same geometries and scenarios. There are a wide selection of dispersion models that are useful for different situations. Here we discuss a chosen set of operational models, i.e., close to real-time models, which have been tested upon several different cases spanning geometries from open field dispersion to the complex geometry of central Paris.

ARGOS

ARGOS is sold by PDC-ARGOS (Denmark) and is an operational commercial software for crisis analysis involving CBRN agents (PDC-ARGOS, 2016). It deals with scenarios such as gas releases (no liquid discharge), fires, explosions and nuclear accidents. The dispersion sub-model Rimpuff is a local scale puff model taking into account local wind variations and turbulence levels. It can also calculate dry and wet deposition. ARGOS includes models for estimating the releases from containers and pipes as well as evaporation of spills on the ground and has also a special model for dispersion of heavy gasses. Heavy gases behave quite different than normal aerosols or smokes from fires. ARGOS can geo-reference a domain and import user specified meteorological profiles, weather profiles from meteorological towers or numerical weather prediction (NWP) data. A database is included for a number of substances. Based on the properties in the chemical database, ARGOS can calculate suggestions for emergency zones based on the levels of concerns for the substances involved in the incident. Obstacles can be taken into account through the sub-model Urban Dispersion Model (URD) which has been used for the Paris scenario. Since ARGOS cannot use URD for dense gas releases, only the neutral gas release has been modelled in the

Paris scenario. For the INERIS case, the heavy-gas module was used for the release of ammonia without any obstacle present, while neutral gas only was released against the obstacle.

QUIC

QUIC (Quic Urban and Industrial Complex) is developed at LANL laboratory, US, and is specifically designed for treating crisis urban scenarios with TICs, C, B and R agents and a number of source terms (Los Alamos National Laboratory, 2016). A material database is not provided, so users have to enter their own material properties. The wind field is computed from a diagnostic mass preserving model. QUIC-PLUME uses Lagrangian random-walk dispersion model, accounting for building-induced turbulence to reconstruct the chemical concentration field. Buildings are constructed either manually, based on simple available geometrical forms, or automatically from imported shape files. Winds can be provided as academic laws or imported discrete data profiles in multiple points. Multiphase releases are also available in addition to basic source terms.

PUMA

The Swedish Defence Research Agency (FOI) develops a custom made program suit for atmospheric dispersion called FOI Dispersion Engine (DE). Several models are included in DE that together span the entire spectrum of temporal and spatial scales needed when dealing with dispersion issues. The model PUMA is designed to operate in real-time and utilizes Gaussian puffs in a Lagrangian approach. The puffs are semi-symmetrical discrete puffs that collectively represent the entire concentration field from one or several sources. In the case of neutral gas the puffs are independent of each other and evolves due to parameterized turbulence as they are transferred according to the meteorological circumstances. PUMA has been extended to also include dense gas physics. The main phenomena that capture the nonlinear dense gas case have been developed and implemented. The introduction of dense gas implies a transition from independent to dependent puffs. Since the main idea with PUMA is to be as fast as possible, the puffs are still treated individually to a high extent. Basically each puff is first treated separately and independently with the inclusion of dense gas physics. In the next step dependencies between overlapping puffs are treated. The model is still under development and the results here represents the model status at the end of 2015.

PMSS

ARIA Technologie is a French company has developed PMSS (Parallel Micro Swift Spray) as a micro-scale version of its own models of wind computation (SWIFT) and agent atmospheric dispersion modelling (SPRAY) (ARIA VIEW, 2016). This version allows for obstacles in a simplified way and performs the dispersion computation in a Lagrangian mode. Obstacles can be isolated or representing a town district. PMSS software is thus constituted by two modules: Micro Swift that computes diagnostic 3D wind field and Micro SPRAY that computes 3D dispersion. It is necessary to pre-process building description files to be readable by PMSS through the translator SHAFT provided by ARIA. A dense gas module exists, but is not at the time available in the version in use at DGA CBRN Defense. It is worth mentioning that PMSS is part of the CERES software (CEA, FR) and also integrated in a HPAC version that is not available in France.

REAL SCALE EXPERIMENTS - INERIS

An outdoor release experiment of ammonia has been conducted at the Centre of Scientific and Technical Studies of Aquitaine (CEA-CESTA) in France. The release site has a radius of approximately two kilometres, is flat and free from any obstacles (Gentilhomme, 2013).

Without obstacle, test #4

Ammonia was released with an average flow rate of 4.2 kg/s through a release device placed on a square (10 m x 10 m) concrete slab, approximately 15 cm thick. The test was a reference case with a horizontal release through a 50.8 mm diameter orifice without any obstacles. The temperature during the test was 12.5 °C, the relative humidity 82% and the wind velocity was 3 m/s at 7 m height. The experiment was simulated using ARGOS, QUIC and PUMA.

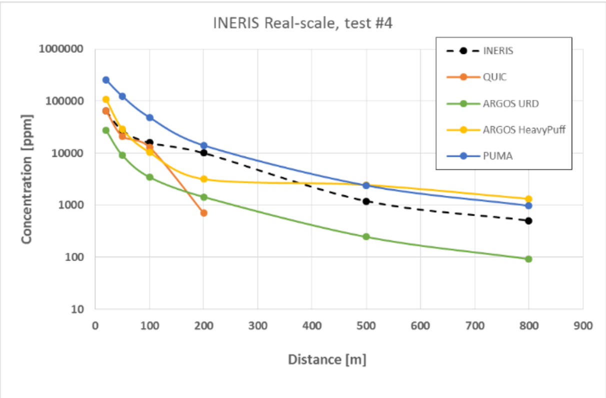

Figure 1. Comparison of experimental and simulation results for the plume centerline concentration at 1.0 meters height above the ground.

Figure 1 shows that the results from the HeavyPuff module in ARGOS are much closer to the measurements done at INERIS than the results from ARGOS using the URD module. This is because compressed ammonia act as a heavy gas close to the release site and this is not captured by the URD module. In this case ARGOS uses the HeavyPuff module up to 440 m from the release site, where Rimpuff takes over. PUMA constantly over-predicts the plume centreline concentration. However, the relative concentration change over distance is quite close to that of the experimental data.

QUIC multiphase pick results are shown for the case without obstacle in orange colour in Figure 1 and in the left panel in Figure 2. The jet horizontal direction is well taken into account (not possible for passive release) and leads to a good correlation in close field (distance <100m). In far field, too much deposition imposed to the model leads to a strong underestimation.

With obstacle, test #5

In this case the jet is obstructed by a concrete wall of dimension 3x3 meters located 3 meters from the source.

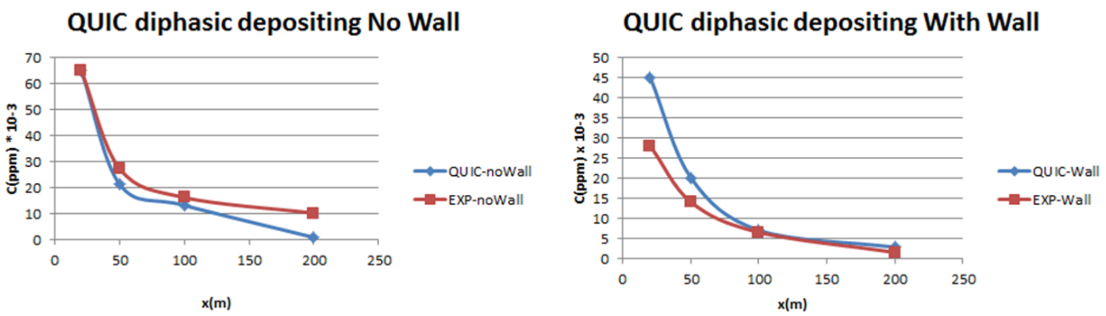

Figure 2: QUIC dense gas release without wall (left) and with wall (right)

In the case with obstacle in the close-field (right panel in Figure 2), the correlation between QUIC and the experiment is not as good as in the no-obstacle case. This is caused by the fact that rainout is not considered in the model. Some dilution by the obstacle takes place (compare with the no obstacle case) and a good far-field correlation is retrieved.

WIND TUNNEL EXPERIMENTS – PARIS

Extensive down-scaled, geometrically by a factor of 350, experiments were conducted at the EnFlo ‘meteorological’ wind tunnel University of Surrey (Robins et al., 2016). Many different cases were investigated using both neutral and dense gases. The most complex case included the urban region of Paris centred on Champs-Élysées. The same geometry was also utilized in a study of operational models and the results are here compared.

ARGOS has been used in full scale for the calculation of the Paris scenario.

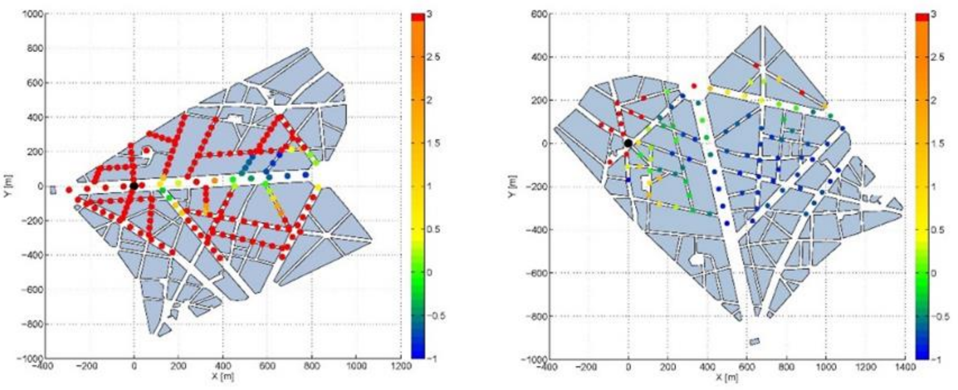

Figure 3. Comparison of ARGOS concentrations with wind tunnel measurements (Source position S1 to the left and S3 to the right). Positive values indicate factors of over-prediction and negative values indicate factors of under-prediction. The black dot shows the position of the source. The wind direction is from left to right in the figures.

Since most of the significant concentrations of air in the wind tunnel from source position S1 are not retained as much as from the other source positions, but channeled along Champs-Élysées, a large portion of the predicted ARGOS concentrations outside Champs-Élysées are higher than in the wind tunnel (left panel in Figure 3). However, the overestimation by Argos upstream of S1 is not significant, as they represent very small concentration values. ARGOS also predicts a faster decrease of agent concentration along Champs-Élysées compared to the wind tunnel, resulting of under-prediction of the air concentration at the longest distances from the source. When the source is located in a more enclosed position (S3), where the wind is not channeled along large avenues, ARGOS produces results more similar to wind tunnel measurements (Right panel in Figure 3).

PMSS has been used for the Paris cases (presented here for source positions S1 for passive gas release). Results are presented as

a) Analysis rates (MOE1=overlapping between experiment and simulation, Occurrence=probability to observe a given concentration)
b) MOE2 indicating performances of false positive (FP) against false negative (FN) rates
c) FAC2 and FAC10 values for individual concentrations and all concentrations

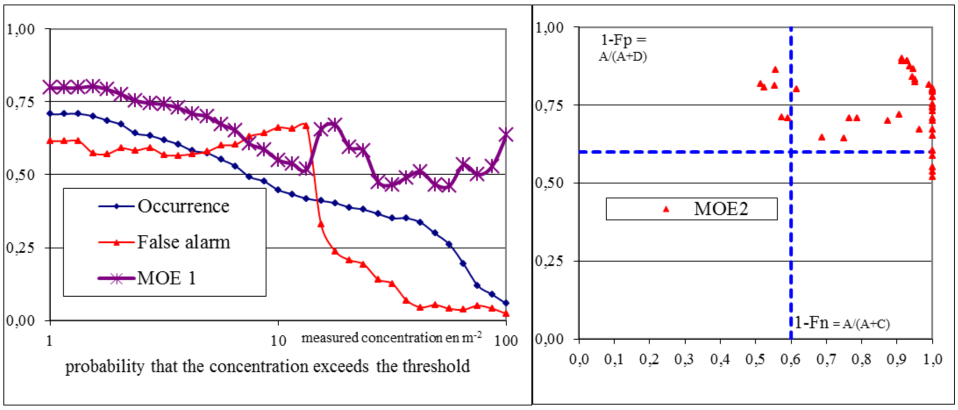

Figure 4. Left panel, false alarm represent ~60% for low concentrations < 10m^{-2} in streets a few hundred meters from the source. Much better False Alarm rates (< 25%) are obtained if we cut at 10m^{-2}. MOE1 > 50% is acceptable for validation purpose. Right panel, points are in general centered in a 60% square. A few false positives and false negatives in far field are probably due to an orientation shift between experiment and simulation.

GENERAL CONCLUSIONS

In this study, we wanted to assess the capabilities of current national members' in-use operational models to handle complex urban dispersion of dense gas release. Referring to COST action ES1006 (COST ES1006 (1), COST ES1006 (2)) on the use of atmospheric dispersion models in emergency response tools, we confirm a number of statements: 1) 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. 2) 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. 3) These models are usually conservative, and overestimate the concentration levels close to the source which may lead to an exaggerated decisions. In addition to these remarks, our current models are not all capable to handle dense gas dispersion, and take into account obstacles or complex geometries.

QUIC software seems to work well using the included dense gas sub-model (compared to INERIS Ammonia release data). The latest developments on PUMA have been tested with promising results in the scope of this project, dealing with dense puff interaction, in a semi-linearized way to keep the response fast enough. PUMA is a real-time model and is not able to treat obstacles and is therefore not suitable for complex geometries. ARGOS heavy puff model also provides good results for dense gas on open field but cannot handle obstacles in combination with dense gas. Regarding obstacles, ARGOS URD model with RIMPUFF puff model is mainly suited to a densely built urban like area but can only handle passive gas. On the PARIS case, tendency to overestimate by a factor of 3 to 5 close to the source, and underestimate by such in far field, was observed and explanations were proposed. PMSS was tested against the PARIS case for passive gas only and behave quite satisfyingly. Overestimations of concentrations behind buildings and underestimations in main streets was usually observed. This semi-operational tools demand some skill to scale and import shape files of the urban area. A dense gas module exists but was not available at the time.

In conclusion, as far as we tested our models, only QUIC has proved able to handle both obstacles and dense gas, PUMA was modified to handle dense gas characteristics but lacks functionalities on urban geometries. PMSS and ARGOS were partially validated with passive gas on urban scenarios, but dense gas module remain to be tested/developed. These models are not push-button tools and require various level of expert skills. The advantage against CFD is their cheap computer cost, but they still need relatively large set-up times compared to the run-time. For a substantially more thorough description of the models and all results we refer to the project report (Burkhart, Gousseff, Tørnes, & Björnham, 2016).

ACKNOWLEDGEMENT

This work was conducted within the European Defence Agency (EDA) project B-1097-ESM4-GP "Modelling the dispersion of toxic industrial chemicals in urban environments" (MODITIC).

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