# Adaptation of three atmospheric dispersion models for jack rabbit ii case study and comparisons with observations : lessons for predictive modelling around industrial sites

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# ADAPTATION OF THREE ATMOSPHERIC DISPERSION MODELS FOR JACK RABBIT II CASE STUDY AND COMPARISONS WITH OBSERVATIONS: LESSONS FOR PREDICTIVE MODELLING AROUND INDUSTRIAL SITES

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**Abstract**: Chlorine release trials were conducted at the Dugway Proving Ground in Utah, during the Jack Rabbit II trials. An interesting database of emissions and dispersion of pressurized liquefied chlorine was set up. This database allows to make comparisons between atmospheric dispersion modelling and large-scale observations about toxic massive releases (up to 10 ton). In this work, three test cases (2 trials free of obstacles and an obstructed environment) were studied on purpose for a model inter-comparison study. INERIS modelled these cases with three atmospheric dispersion models: the open source SLAB code, the commonly used PHAST software (commercial licence) and the 3D code FDS (Fire Dynamic Simulator). This paper focuses on the adaptation of the models and comparisons with observations in the near-field for CFD (Computational Fluid Dynamics) modelling and large field (up to 10 km) for other models. Discussions about harmonization of practices between models and practices for toxic consequences assessment around industrial sites are also proposed. Indeed, a massive release of pressurized liquefied material could generate complex phenomena around the release location: jet under pressure, rain-out, cooling, etc. For each of these atmospheric dispersion models, the source term can be set up in various ways depending on its level of complexity. A similar discussion is proposed about the unsteady meteorological flow that cannot be assessed by the simplest models.

***Key words:*** *Jack Rabbit II, chlorine field experiment, dense gas models, model validation*

## INTRODUCTION

During the Jack Rabbit (JR) experimental campaigns (JR I in 2010 and JR II in 2015 and 2016) series of chlorine releases have been performed at Dugway Proving Ground (DPG) in Utah. Further details of the trials have been already presented in various presentations and publications (e.g. Fox *et al.*, 2017). An original dataset has been developed that is valuable for which had concern in the possible effects of pressurized liquid chlorine releases such as storage tanks and transportation vessels (e.g., see Hanna et al. 2016). An intercomparing modelling exercise was launched in March 2018, coordinated by Tom Mazzola (Engility Corporation), Steven Hanna (Hanna Consultants) and Joseph Chang (RAND Corporation). Three

of the nine Jack Rabbit II experiments were selected for the initial phase of the inter-comparison exercise and harmonized inputs were delivered to participants. The mass of pressure-liquefied chlorine released in the trials 1, 6 and 7 was respectively 4.5 tonnes, 8.4 tonnes and 8.6 tonnes. For Trial 1, a grid of Conex shipping containers was set up around the release point to simulate an urban array of buildings. For Trial 6 and 7 the grid of Conex was removed so that the release was performed in a free field environment. In Trials 1 and 6, the released jet was directed vertically downwards onto a concrete pad from a height of 1 m. In Trial 7, the jet was angled 45-degree downwards from the horizontal. Arc concentration sensors were set up downwind from the release point at various distances up to 11 km.
The main topic this paper is the evaluation of 3 atmospheric dispersion models (SLAB, PHAST, FDS), based on strongly different approaches, by comparison with experimental data. The different characteristics of those models also offer the opportunity to discuss about harmonization of the practices for atmospheric dispersion modelling for unobstructed environment.

## 3 MODELLING APPROACHES

The first model that was run is the widely-used dense gas dispersion model SLAB. This model allows to simulate a ground-level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet, and an instantaneous volume source dispersion. All these types of sources, except for evaporating pool, could handle releases with gaseous form or liquid form or a mixture of vapor and liquid droplets. The vapor-droplet mixture is treated as a monophasic fluid where droplet rain out and soil deposition are neglected. SLAB is able to handle dense gas dispersion but is not able to handle both evaporating pool and jet. The atmospheric dispersion is then computed based on heavy gas cloud collapse and is then based on the resolution of simplified equation of fluid mechanics.
PHAST software is a calculation tool dedicated to model the effects of accidental hazards related to industrial activities. The atmospheric dispersion model of this software is of the "integral" type. Such type of model used a simplified resolution of fluid mechanic equation in the near field, solved along the curvilinear abscises of the jet, then dispersion is dealt with a Gaussian approach while the gas density becomes close to the ambient one. The complexity of this type of model is intermediate between Gaussian dispersion calculations for passive gases and three-dimensional software. It allows taking into account the different dispersion regimes. Indeed, it includes several sub-models corresponding to many different issues, such as pressurized gas jets, heavy gas dispersion and a gaussian dispersion model in the far field.
The 3D runs were achieved with FDS (Fire Dynamic simulator), a freely available CFD (Computational Fluid Dynamics) code provided by the NIST (National Institute for Standard and Technology) (McGrattan, 2005). FDS was initially dedicated to model low velocity flow with density gradient such as smoke dispersion modelling in case of fire. Turbulence model is based on the Large Eddy Simulations (LES) approach that consists in the segregation between large scales, explicitly resolved, and small ones, modelled. The key criteria for such an approach is both to ensure that resolved scales are small enough, typically in the inertial zone of the turbulence spectrum, and that energy transfer between productive large scale and dissipative small ones is well modelled. Since the atmospheric turbulence anisotropy is contained in the largest scale and considering small scales are isotropic, this consequently enables solving the whole characteristics of turbulence in the atmospheric boundary layer. Unlike SLAB and PHAST, this tool does not require any assumptions about the orientation with respect to the direction of the wind.

## INPUT PROVIDED FOR MODELLING

The chosen trials reproduce realistic massive releases where numerous physical phenomena can occur. For these trials, the main physical phenomena identified are the following: discharge conditions, interaction between the jet and the pad, pool formation and evaporation, thermodynamics of the cloud, interaction between the cloud and the ground including dry deposition, atmospheric conditions. Discharge conditions, pool formation and evaporation (Spicer and al., 2018), and atmospheric conditions were investigated. Harmonized inputs were provided before running the simulations, they are reproduced in Table 1.

## SLAB MODEL SET UP

Since the source term is complex, SLAB cannot handle simultaneously with the whole different contribution of the source term, various configurations were studied to highlight the sensitivity of source term set up. Two approaches are presented below:

- SLAB_1: The baseline corresponds to a horizontal jet release; the discharge period is equal to the primary release modified for rain out discharge; several averaging times have been tested.
- SLAB_2: all the mass, both liquid and vapour, indicated is considered as an instantaneous release.

The liquid fraction is taken to be consistent with the liquid mass fraction deducted from Table 1. The mean velocity wind profile is reconstructed with power function using the Monin length and surface roughness as input.

Table 1 : Source and meteorological conditions provided to participants of the Jack Rabbit II model inter-comparison exercise. Coloured values indicate the following: **red** = Used for SLAB, PHAST and FDS input; **gray**: used by FDS and SLAB; **orange** = used for FDS validation; **Blue** = used by PHAST; **Green** = calculated internally by SLAB, PHAST and FDS.

| ***Release Parameters*** | **Trial 1** | **Trial 6** | **Trial 7*** |
|---|---|---|---|
| Primary release | | | |
| Discharge rate (kg/s) | 145 | 168 | 162 |
| Discharge period (s) | 20.4 | 32.4 | 33.6 |
| Temperature (°C) | -37.3 | -37.4 | -37.4 |
| Vapor fraction (ignoring KE effects) | 0.264 | 0.266 | 0.274 |
| Density (kg/m$^3$) | 11.89 | 11.79 | 11.41 |
| Velocity (m/s) | 50.8 | 44.2 | 44.2 |
| Area (m$^2$) | 0.24 | 0.323 | 0.322 |
| Evaporated rainout | | | |
| Discharge rate (kg/s) | 43.2 | 34 | 34 |
| Discharge period (s) | 36.8 | 86.4 | 93.4 |
| Temperature (°C) | -37.3 | -37.4 | -37.4 |
| Vapor fraction | 1 | 1 | 1 |
| Density (kg/m$^3$) | 3.16 | 3.152 | 3.144 |
| Area (m$^2$) | 491 | 491 | 491 |

| ***Weather conditions*** | **Trial 1** | **Trial 6** | **Trial 7** |
|---|---|---|---|
| Atmospheric pressure (mbar) | 873.7 | 871.1 | 868.5 |
| Initial wind speed (m/s) at z = 2 m | 1.45 | 2.42 | 3.98 |
| Initial wind direction at z = 2 m | 147.4 | 146.9 | 149.6 |
| Initial temperature (°C) at z = 2 m | 17.5 | 22.3 | 18.7 |
| Surface roughness (mm) | 0.5 | 0.5 | 0.5 |
| Friction velocity, u* (m/s) | 0.108 | 0.093 | 0.210 |
| Sensible heat flux, Hs, (K-m/s) | -0.012 | -0.0034 | -0.0160 |
| Vertical profiles of wind speed and direction and temperature | | | |
| Inverse Monin-Obukhov length (m$^{-1}$) | 0.124 | 0.056 | 0.0229 |
| Pasquill Class | E/F | E | D/E |

## PHAST MODEL SET UP

Various configurations have been used:

- PHAST_1 : input directly from specification given to the modelers (see Table 1) for TRIAL 1, 6 and TRIAL 7; (PHAST_1_E refers to Pasquill class E)
- PHAST_2: (for TRIAL 6) impinging jet and rain out computed by the dedicated PHAST sub-model of a line rupture with presence of a bund having a surface equal to the surface pad one.

The mean velocity wind profile was reconstructed thanks to a power function using Pasquill stability class and roughness as input.

## FDS MODEL CONFIGURATION

The numerical domain was 300 m long, 200 m width and 30 m height. Due to several steps of validation required for CFD modelling, trial 6 and 7 were studied in priority. The domain is lined up with the direction of the release. The computational grid is made of 31 million hexahedral elements. The smallest cell length is 0.25 m corresponding to cells located close to the ground. A sufficiently refined mesh near the ground is recommended for FDS to represent properly the wall function. After several tests this thickness has been deemed as the better compromise between accuracy and efficiency. The top of the domain was an open condition and periodic boundary conditions were applied at the edges and outlet of the domain. Regarding the meteorological flow, the key issue consists in prescribing relevant velocity profile in terms of instantaneous velocity. Several approaches were previously tested (Leroy et al., 2016):

- the wind velocity signal in time for FDS inlet boundary condition is obtained by performing a Fourier analysis in time on the experimental signal;

- the SEM methods (Jarin et al. 2008);
- boundary periodic wind with profile reconstruction using Dyer similarity functions using the Monin length and roughness as input.

The FDS results in the present work uses the last approach, already tested on LNG trials (Luketa, 2018). To represent a relevant boundary layer, the wall function must match (Blocken et al., 2007) to the velocity profile, set up by a log law in FDS with aerodynamic roughness), by adjusting the ground grain roughness. A preliminary simulation of the meteorological flow is carried out to obtain a meteorological fully developed flow before the release to be modelled. Several tests and adjustments have been performed to reach levels of turbulence close to observations done just before the release. The comparison of the modelled flow with observed at first experimental levels is satisfactory as far as the mean velocity is concerned. The comparison of some FDS results with observed turbulence is presented in Table 2 for TRIAL 6. There is quite good agreement for this first sets of simulation. Further tests highlight the importance in accounting for the sensible heat flux to simulate stable conditions. The evaporating rainout has been simulated by an emissive surface equivalent to the pad surface, with the gaseous mass flow rate presented in Table 1. The source term of the jet has been set up by a gaseous release. No deposition was considered.

Table 2 : Recommended u* and turbulence for modeling provided to participants of the Jack Rabbit II model inter-comparison exercise and results obtained by FDS at the location of the release source for TRIAL 6

| | u* | $\sigma_{hor}$ | $\sigma_{hor}$/u* | $\sigma_w$ | $\sigma_w$/u* |
|---|---|---|---|---|---|
| Observations | 0.093 | 0.416 | 4.824 | 0.647 | 1.161 |
| FDS_I | 0.141 | 0.311 | 2.210 | 0.133 | 0.941 |

## RESULTS

The centerline concentrations obtained are presented in **Figure 1** and in **Figure 2**. Regarding SLAB results, for TRIAL 6, the puff instantaneous release (SLAB_2) case gives the highest concentrations in the near field. Sensitivity with averaging time is observed in the near field.

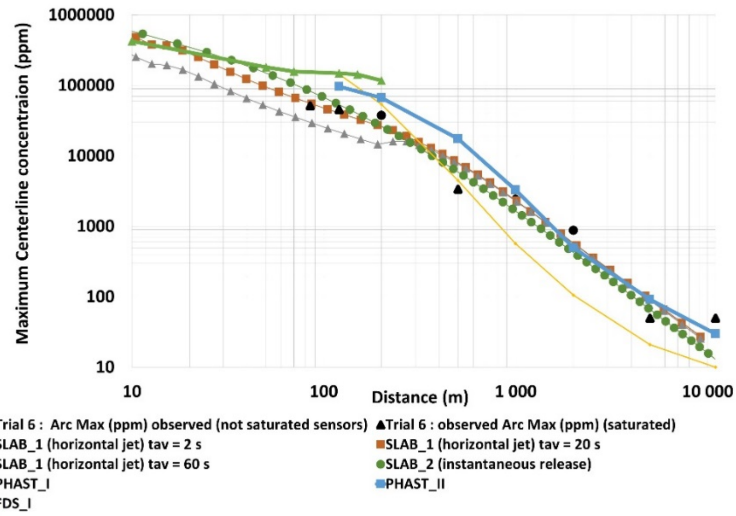


**Figure 1.:** Maximum arc-wise concentrations obtained for TRIAL 6

Comparisons as a whole for TRIAL 6 and 7 do not show an overestimation for the SLAB and PHAST results. Other source term configurations could be tested but for emergency situation it is worth bearing in mind this preliminary trend. Comparisons appear in a better concordance for TRIAL 1, not plotted here. No conclusion regarding the physics can however be done about models' performance since obstacles were ignored. Regarding the FDS results, the decrease of concentration downwind differs from previous models due to the fact that the FDS approach enable taking into account the interaction between the jet and the ground. Indeed, in the near field the recording video (http://www.uvu.edu/esa/jackrabbit/) show the cloud dilution and coherent turbulent structures. It would be desirable to validate this issue for CFD modelling. FDS results seem very conservative, but this is consistent with the physics taken into account at this stage, where droplet interaction with the ground and deposition on the ground were ignored.

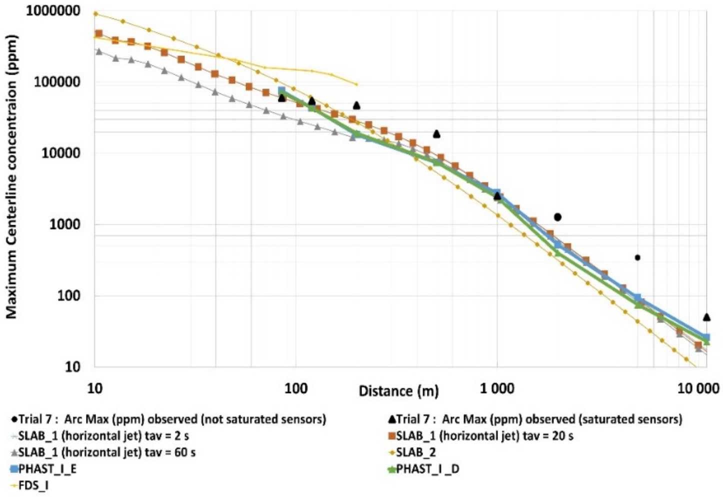


**Figure 2.:** Maximum arc-wise concentrations obtained for TRIAL 7

## CONCLUSIONS

The methodology to model JR II trial cases with SLAB, PHAST and FDS was discussed. Several configurations to assess emissive source term were presented for SLAB and PHAST. Results were compared with observed maximum centreline concentrations. Comparisons as a whole for TRIAL 6 and 7 do not highlight an overestimation for the SLAB and PHAST results. FDS ones indicate a decrease of the centerline concentration that differs with others. In the FDS model, one of the key phenomena, i.e. the interaction between the momentum of the jet and the ground, is more precisely modelled. This capability of CFD codes to consider obstacle effects in the atmospheric dispersion process should be more deeply investigated.


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