**Software used for the simulations**: ADAM (Version 3.0)

The Accident Damage Analysis Module Software (ADAM) is an official tool of the European Commission [1] designed to support environment, safety and civil protection authorities tool for estimating the consequences industrial accident in terms of thermal radiation, overpressure or toxic concentration that may result from an unintended release of a flammable or toxic substance [2-5]. For this purpose, suitable models were selected and combined to aid in simulation of the possible evolution of an accident, from the time of release to the final damage. The evaluation of the tool performance is reported in [3], and [4].

With reference to airborne dispersion, the model implemented in ADAM is based on SLAB [6]. Amongst the several code improvements of the original model the following model modifications have been implemented in ADAM (for more details see [2],and [5]: (i) alternative calculus of the average concentration for instantaneous releases; (ii) inclusion of the source term module by addressing time-varying releases; (iii) calculus of the rainout; (iv) combination of the contribution from direct vapour source and from the pool vaporization in case of rainout; (v) Calculus of downward jets dispersion by including modifications to the rainout module.

The current simulations were carried out by using the model input conditions given in Table 1 of “Jack Rabbit III Modelers Working Group Initial Modeling Exercise (2021-2022)”, Version 2.3, 21 December 2021 by Joseph Chang and Simon Gant. The source term module of ADAM was partially bypassed by using a constant release rate and the release duration as given in Table 1. By contrast the rainout and the following evaporation were calculated using the ADAM calculus library. This allows estimating the mass fraction of the droplets falling on the ground and those remaining airborne, and the dispersion is calculated by using a recombination algorithm (see [2]). In particular, the dispersion effect of the vapour jet is combined with the vapour resulting from the vaporisation of the rainout pool. These two phenomena are considered as independent, and ADAM separately estimates the effects associated with each other. The overall concentration is conservatively estimated by adding up each contribution after having applied the ADAM-SLAB model twice. The first calculus is conducted on the primary phenomenon i.e., the one associated with the direct vapour jet, whilst the second is associated with the secondary and less relevant phenomenon (i.e., the vaporisation for the pool resulting from the rainout).

For both Desert Tortoise and FLADIS experiments, according to ADAM simulations all aerosols components evaporated or rained out before the position of the closest sensors (i.e. 100m and 20m, respectively). The output data refer to the vapour concentration only.

For Desert Tortoise the calculated rainout was lower than the value of 5% proposed on Table 1. It resulted indeed of less than 1%, on average. For FLADIS, no significant pool was determined, and in this case the recombination procedure was not required.

Averaging time was applied as indicated in Table 1 of the aforementioned report.

The following section provides the list of files containing the ADAM simulations. The first series of files provides the predicted arc-max concentrations versus distance for all six trials given in Table 1, at 1m height from the ground. The second series of files give the predicted plume widths calculated from the moments of the concentration distribution across the arc of sensors (CERC, 2000). Together with the plume widths arc-max concentrations for the different arc distances and heights were given. This to allow a better punctual comparison with the experimental data, that is particular relevant for FLADIS trials where the sensor were positioned at different heights.

**Results of ADAM simulations**

The outcome of ADAM simulation for both Desert Tortoise and FLADIS is given hereunder:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| *Desert Tortoise* | | | | | |
|  | **Distance** | **Height** | **DT1** | **DT2** | **DT4** |
| **Arc-Max Concentration (ppmv)** | 100 m | 1 m | 117113 | 154476 | 143548 |
|  | 800 m | 1 m | 6385 | 10553 | 12352 |
| **Plume Width(m)** | 100 m | 1 m | 12,5 | 13,9 | 15,2 |
|  | 800 m | 1 m | 73,7 | 101,5 | 122,7 |
| *FLADIS* | | | | | |
|  | **Distance** | **Height** | **FLADIS9** | **FLADIS16** | **FLADIS24** |
| **Arc-Max Concentration (ppmv)** | 20 m | 0,1 m | 20360 | 18083 | 19773 |
|  | 70 m | 0,5 m | 2268 | 2128 | 1463 |
|  | 238 m | 1,5 m | 240 | 267 | 140 |
| **Plume Width(m)** | 20 m | 0,1 m | 1,9 | 2,5 | 2,4 |
|  | 70 m | 0,5 m | 6,6 | 8,0 | 7,6 |
|  | 238 m | 1,5 m | 19,1 | 20,2 | 21,1 |

**ADAM RELATED FILES**

1. DESERT TORTOISE

**ADAM\_centreline\_DT1.csv**

**ADAM\_centreline\_DT2.csv**

**ADAM\_centreline\_DT4.csv**

Thesefiles contains semicolon-separated data with the maximum near-ground (i.e. 1 m height) concentration (ppmv) vs. downwind distance (from 10 to 1000 m). Concentrations were calculated at a fixed height of 1 m, which corresponds to the location of the sensors.

**ADAM\_arc\_conc\_width\_DT1.csv**

**ADAM\_arc\_conc\_width\_DT2.csv**

**ADAM\_arc\_conc\_width\_DT4.csv**

Thesefiles contains semicolon -separated data with:

*First column*: arc distance (i.e., 100m and 800m)

*Second column*: maximum concentration at 1m height at these arc distances

*Third column*: plume width, 𝜎𝑦, from the moments of the concentration distribution across the

arc of sensors (CERC, 2000) at these arc distances

1. FLADIS

**ADAM\_centreline\_FLADIS09.csv**

**ADAM\_centreline\_ FLADIS16.csv**

**ADAM\_centreline\_ FLADIS24.csv**

Thesefiles contains semicolon-separated data with the maximum near-ground (i.e. 1 m height) concentration (ppmv) vs. downwind distance (from 10 to 1000 m). Concentrations were calculated at a fixed height of 1 m, which is in between the location of the sensors for the different arc-distances (i.e., 0.1, 0.5, 1.5).

**ADAM\_arc\_conc\_width\_ FLADIS09.csv**

**ADAM\_arc\_conc\_width\_ FLADIS16.csv**

**ADAM\_arc\_conc\_width\_ FLADIS24.csv**

*First column*: arc distance (i.e., 20m, 70m and 238m)

*Second column*: maximum concentration at heights: 0.1m (for arc 20m), 0.5m (for arc 70m) and 1.5m (for arc 238m)

*Third column*: plume width, 𝜎𝑦, from the moments of the concentration distribution across the

arc of sensors (CERC, 2000) at these arc distances

**References**

[1] 2017. Commission Decision of 29.8.2017 Regarding the Distribution of the Software Accident Damage Analysis Module (ADAM). Brussels, 29.8.2017 C 6012 final.

[2] Fabbri, L Binda, M Bruinen de Bruin, Y; Accident Damage Analysis Module (ADAM) – Technical Guidance, EUR 28732 EN, Publications Office of the European Union, Luxembourg, 2017, ISBN 978-92-79-71879-3, doi 10.2760/719457, JRC107633.

[3] Fabbri, L Binda, M and Wood, M; Evaluation of the Accident Damage Analysis Module (ADAM) tool - Verification and Validation of the implemented models in ADAM for Consequence Analysis, EUR 29363 EN, Publications Office of the European Union, Luxembourg, 2018, ISBN 978-92-79-94668-4, doi:10.2760/582513, JRC113187.

[4] Fabbri, L and Wood, M; Accident Damage Analysis Module (ADAM): Novel European Commission tool for consequence assessment—Scientific evaluation of performance. Process Safety and Environmental Protection, Volume 129, September 2019, Pages 249-263.

[5] Fabbri, L Wood, M Azzini, I Rosati, R; Global sensitivity analysis of the ADAM dispersion module: Jack Rabbit II test case. Atmospheric Environment, Volume 240 (2020) 117586

[6] Ermak D.L., (1990), “User’s manual for SLAB: an atmospheric dispersion model for denser-than-air releases”, Lawrence Livermore National Laboratory, Livermore, California, UCRL-MA-105607