TECHNICAL NOTE

Notes on FLADIS and Desert Tortoise simulations

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1 Equivalent source

FLACS-CFD (FLACS) cannot simulate two-phase releases, therefore we use an equivalent gas-phase source.
Two different equivalent sources are used: one is the provided equivalent source (CERC), and one is an equivalent source that is calculated using a utility program in FLACS. The FLACS utility requires the stagnation pressure as input. For Desert Tortoise, this is provided in the experiment report. For FLADIS, the stagnation pressure is assumed to be given by the sum of the static pressure and the dynamic pressure at the orifice and so we calculate the dynamic pressure from the orifice area, measured mass rate and density of liquid ammonia at the measured release temperature. The FLACS utility also requires the relative turbulence intensity and the turbulence length scale for the source. We follow the user guidelines and set the relative turbulence intensity to 2% and set the turbulence length scale to 10% of the equivalent source diameter.
The equivalent-source calculation in FLACS predicts a rainout rate of less than 0.5% of the total mass rate. The equivalent source is assumed to describe the plume at a downstream location where all the liquid ammonia has evaporated, and no rainout or pool evaporation are included in any of the simulations, using the provided or the calculated equivalent sources.

	FLADIS 9		**FLADIS 16**		**FLADIS 24**	
	FLACS	**CERC**	**FLACS**	**CERC**	**FLACS**	**CERC**
Downstream distance (m)	4.8	4.2	3.0	3.1	4.8	4.4
Velocity ($m\ s^{-1}$)	3.85	4.75	4.34	5.12	3.30	4.22
Density* ($kg\ m^{-3}$)	1.64	1.67	1.64	1.64	1.64	1.64
Temperature (deg C)	-68.80	-69.45	-68.51	-69.25	-68.75	-69.15
Diameter (m)	1.34	0.88	0.83	0.73	1.33	1.06
Mass concentration ($kg\ kg^{-1}$)	0.07321	0.07056	0.07481	0.07056	0.07350	0.07057

Table 1. FLADIS: provided and calculated equivalent source terms.
**Density is not required by FLACS for definition of the equivalent source but is provided here so that the terms can be compared more fully. Note that mass concentration was calculated for the provided equivalent source terms from the molar concentration, taking into account the ambient humidity.*

	DESERT TORTOISE 1		**DESERT TORTOISE 2**		**DESERT TORTOISE 4**	
	FLACS	**CERC**	**FLACS**	**CERC**	**FLACS**	**CERC**
Downstream distance (m)	55.0	51.0	64.2	48.3	62.5	49.5
Velocity ($m\ s^{-1}$)	5.32	7.50	5.46	6.00	5.62	8.59
Temperature (deg C)	-66.87	-68.15	-66.76	-68.15	-66.34	-68.15
Area (m^2)	176.04	80.80	239.13	140.98	225.57	97.24
Molar concentration (-)	0.136	0.130	0.137	0.130	0.141	0.143

Table 2. Desert Tortoise: provided and calculated equivalent source terms.

2 Notes for FLADIS simulations

2.1 Steady-state solver

Some buildings upstream of the release were noted to have impacted the plume and are therefore included in the simulations, creating a very large domain. This, and the long duration of the releases, makes the simulations computationally expensive when the transient solver is used.
To reduce the computation time, we run steady-state simulations, which is reasonable, given:

- Figure 13 in Nielsen et al. (1997) is a timeseries plot of concentration measured at a fixed distance from the release and shows that a state is reached in which the variation of the concentration is limited to high-frequency turbulent fluctuations. The experiment for this timeseries is not included in the present modelling exercise but the conditions and experimental setups were similar for all the FLADIS trials.
- The measurements from which the maximum concentrations were calculated were moving-averages for windows of 600 s (FLADIS 9 and FLADIS 16) and 400 s (FLADIS 24). These windows are shorter than the release periods (900, 1200, and 600 s for FLADIS 9, FLADIS 16 and FLADIS 24, respectively) and so we can be reasonably confident that at least one averaging period would include only data from the steady-state stage in a transient simulation.
- The wind speed, and the time required for the plume to be transported to the furthest downstream measurement point (238 m), relative to the duration of the release and duration of the averaging window, means that we anticipate steady-state conditions would last for at least the duration of the averaging window at 238 m in a transient simulation.

2.2 Caveats to simulations

The downstream distance for the equivalent source is interpreted as a distance in the release direction, since any deviation from this (e.g., due to misalignment of the wind direction) is likely to be small within the first few metres from the source. Since no height is provided for the equivalent source term, the height was assumed to be equal to the release height (1.5 m for all experiments) and the equivalent source is modeled as circular.
FLACS requires the mean surface heat flux (the vertical heat flux from the ground to the air) to simulate unstable atmospheric conditions, such as the Pasquill Class C conditions in FLADIS 24. This was calculated following Golder (1972), using the provided relative humidity and air temperature to calculate the specific heat capacity and density for the air:

mean surface heat flux = $(u^*)^3 \times C_{air} \times \rho_{air} \times T_{air} / (k \times g \times MO)$

u^* : friction velocity (provided)
C_{air} : air specific heat capacity
ρ_{air} : air density
T_{air} : air temperature (provided)
k : von Karman constant
g : gravitational acceleration
MO : Monin Obukhov length (provided)

2.3 Grid resolution

We set the grid resolution such that the equivalent source diameter was resolved by 20 grid cells, and beyond this region, cells were stretched, i.e., cells became larger as distance from the equivalent source increased. The maximum size ratio between neighbouring cells was set to 1.2 and the maximum cell size was set to 10 m.

3 Notes for Desert Tortoise simulations

3.1 Grid and domain choice

The domain size and grid are made by guessing the plume shape and considering the distance of interest for ammonia concentrations. A grid sensitivity is performed by (i) increasing the resolution in the vertical direction in the region close to the ground from 0.25 m to 0.15 m and (ii) increasing the extent of the horizontal fine-resolution region starting at the source and extending downstream (where the cell size is as fine as 1 m). For the three grid setups, the variation of simulated maximum concentration at different distances from the release is hardly visible when plotted in the range from zero to the concentration at the equivalent source.

3.2 Aspect ratio of the equivalent source

The area of the recommended vapour-only equivalent source has aspect ratio of 5. An additional set of simulations is defined changing the aspect ratio of the equivalent source to 2.

3.3 Shape of the equivalent source

A flat profile is chosen for velocity and concentration at the equivalent source.
Observations and measurements from the experiments suggest that the concentration in the plume was decreasing moving from the centre to the sides. FLACS allows to define a parabolic profile of velocity at the source, this option is used as alternative to the baseline flat profile in a set of simulations to obtain a non-uniform concentration flux with maximum value at the centre and zero flux at the edges of the rectangular source region.

4 Post-processing

The maximum concentration was calculated at 1 degree intervals along arcs at fixed distances from the release, for heights at 0.02 m intervals between 0 and 3 m above the ground. The maximum value from these was taken to be the maximum concentration at each horizontal arc-distance. The FLADIS experiments are simulated as steady state scenarios and so no time averaging is required. For Desert Tortoise, the simulated concentrations are time-averaged by applying a moving time-window, as was done for measured concentrations, and the maximum arc-wise concentrations are calculated from the time-averaged values.

4.1 Files with results from FLADIS simulations

FLADIS_arcmax_concentrations_flacs.txt: results from the simulations using the FLACS equivalent source
FLADIS_arcmax_concentrations_cerc.txt: results from the simulations using the provided equivalent source
Simulations using both Pasquill classes for FLADIS 16 and FLADIS 24 are included in the results files since these experiments took place in borderline conditions.

4.2 Files with results from Desert Tortoise simulations

Results of each simulation are provided in a separate file. The file name describes the scenario in the format:
<test>-<equivalent source>-<aspect ratio>-<profile>.csv
where:
test = **DT1 | DT2 | DT4**
equivalent source = FLACS **| CERC**
aspect ratio = 2 **| 5**
profile = **flat |** parabolic

Values in bold identify the baseline scenario. For scenarios with aspect ratio=2 only the case profile=flat is simulated while the case profile=parabolic is omitted.

5 References

Golder, D. Relations among stability parameters in the surface layer. *Boundary-Layer Meteorol* **3,** 47–58 (1972). https://doi.org/10.1007/BF00769106.
Nielsen, M. et al. Field experiments with dispersion of pressure liquefied ammonia. *Journal of Hazardous Materials* **56**, 59-105 (1997).