Dispersion Calculations for Jack Rabbit III Modelling Exercise

# Code

Calculations were carried out in Shell FRED 2022. FRED can access the following internal models for release and dispersion:

* GENREL: a model to calculate release and initial expansion/flashing for liquid, gas and two-phase releases
* AEROPLUME: a model for gas dispersion for situations starting with a gas or two-phase jet.
* HEGADAS: a model for dispersion of ground level passive (i.e. non momentum-driven) gas releases typically, but not necessarily, from a pool.
* PGPLUME: a Gaussian dispersion code for passive dispersion.

It is possible for dispersion calculations to transition from one model to another. Typical transitions are from AEROPLUME to HEGADAS or AEROPLUME to PGPLUME. However, AEROPLUME contains entrainment functions applicable to both dense and passive dispersion so that calculations which begin with AEROPLUME can remain within that code.

As the concentration predictions were not sensitive to model transitions, for simplicity AEROPLUME has been used exclusively for the results presented. As FRED allows users the choice of only instantaneous and 600 s averaging times, the AEROPLUME results have been processed in Excel to produce data at the required averaging times.

# Notes & Deviations from Requested Data

All calculations begin at the release point. The expansion to atmosphere together with the resulting liquid fraction is calculated by FRED. Hence the equivalent source conditions provided as part of the exercise documentation for the Desert Tortoise and FLADIS trials are not used.

In normal use, process conditions are provided to FRED and FRED will calculate mass flow rates from relatively simple rule set designed to be consistent and conservative. For the calculations carried out here the mass flow rates were set to the provided values. In all cases this resulted in two-phase exit conditions with a very high liquid fraction. For the FLADIS experiments, the flash fraction after expansion to atmosphere was in good agreement with the data presented in the Modelling Exercise document.

The AEROPLUME model does not allow rain out of liquid and for the Desert Tortoise trials the full mass flow rate remains within the plume at each downwind station. The mass flow rate could be reduced to allow for rain out, but this has not been done so far.

Atmospheric pressure in FRED is set to 1.01325 bar for dispersion calculations, so that the atmospheric pressure in the Desert Tortoise trials is not matched. The functionality to deal with reduced atmospheric pressure exists in AEROPLUME but is not accessed from FRED. A calculation for DT1 was carried out in AEROPLUME directly to test the effect of this. On a logarithmic scale a difference was observable beyond around 400 m but was small. At 800 m one result (for unprocessed ‘top-hat’ concentration) was 0.5% v/v while the other was 0.46% v/v – i.e. around an 8% discrepancy. The effect on expanded velocity was found to be negligible.

For some trials, the averaging time is a large fraction of the release time. This not considered an advisable approach for two reasons. Firstly, the resulting average could be affected by the rise and fall of concentration – i.e. genuinely transient effects may be present. Secondly, the average could be different in a second instance of the same test – one would like an ensemble of results from which to extract an average. e.g. for DT1 it is not known if this is a ‘high’ value for an 80 s average or a ‘low’ value as the release time is only 126 s. In any case, averaging has been allowed for purely using the normal power of -0.2 law – all calculations are steady state.