VDI Guideline 3783 Part 1 is a gaussian Model for the dispersion of neutrally buoyant gases or gases lighter than air.

VDI Guideline 3783 Part 2 is based on systematic experimental investigations of dense gas dispersion in a wind tunnel.

Part 1 and 2 have to be combined when calculating concentrations below 1 Vol.% as this is the case for toxic release thresholds.

AUSTAL (Austal2000) is a langrangian atmospheric dispersion model for simulating the dispersion of air pollutants in the ambient atmosphere. It was developed by Ingenieurbüro Janicke, Germany under contract to the Federal Ministry for Environment, Nature Conservation and Nuclear Safety.

Although not named in the TA Luft, it is the reference dispersion model accepted as being in compliance with the requirements of Annex 3 of the TA Luft and the pertinent VDI Guidelines. The langrangian model itself is described in the VDI Guideline 3945 Part 3.  
  
Austal is also the designated successor of the gaussian Model in the VDI 3783 Part 1. In it’s actual state the VDI 3783 Part 1 is being reviewed with the aim of “modernizing” it, by introducing the langrangian model (of wich austal is an implementation) instead of the gaussian model.

Both, the gaussian and langrangian model as described in VDI 3783 Part 1 are coupled with the (unchanged) VDI 3783 Part 2 for calculating the heavy gas dispersion.

In Austal the heavy gas dispersion is therefore only “implicit” and the explicit concentration values should not be used above 10 Vol.% for the heavy gas dispersion.

Neither gaussian nor Langrangian are able to account for releases with an explicit momentum. Therefore, the calculation differs here form the real case, as the mass flow is released through a “point source” and considered as momentum free / passive dispersion source. This leads to much higher concentrations close to the source.

Other Boundary conditions that **were NOT considered** due to the available BC of the models:

* Atmospheric pressure (is always 1.013 Bar)
* Exit temperature of the Ammonia (could only be considered for the gaussian case)
* Rain out fraction
* Friction Velocity
* Relative humidity
* Deviance of the main wind direction from the main sensor axis
* Any kind of release velocity
* Equivalent source conditions
* Buildings
* Averaging time (all shown concentrations are “stationary” values / the highest values at the considered locations)

For all calculations Pasquill stability Class D (or similar neutral atmosphere) was considered. The Pasquill stability only exists as a BC in Austal. For the VDI 3783 there are only stable/neutral/unstable atmosphere as BC, and Neutral corresponding the Pasquill D.

For the VDI 3783 Part 2 calculations the dispersion area chosen was “Dispersion Area I: flat terrain”.  
  
Whilst AUSTAL enables us to define the wind speed at a varying reference height (therefore Austal Simulations were done with the wind speed and reference heights defined in Table 1 of the “JRIII initial modeling exercise description v2.3”) while in the VDI 3783 Part 1 the wind speed is always to be given at a reference height of 10 m. Therefore the Wind speeds in 2 m height were converted to a reference height of 10 m using a power law wind profile, with an exponent of 0,28 according to the definitions of the Guideline.

The surface roughness chosen was “extremely flat (0.02m)” for DT and FLADIS for the VDI 3783 Part 1. For the calculations with AUSTAL the surface roughness for DT was 0.01m and for FLADIS 0.05m.  
  
I also attached some cross sectional concentration plots (out of AUSTAL) at a distance of 100 m from the source for the Desert Tortoise cases to be compared with the profiles Fig. 7 and Fig. 8 of “JRIII MWG Aspect Ratio for Desert Tortoise v1.0”.

Calculated wind Speed in 10 m height for Desert Tortoise for the VDI 3783 Part 1 calculations:

DT1: given wind speed 7,42 m/s in 2 m height results in 11,64 m/s in 10 m height using a power law with an exponent of 0,28

!!!!!!!!!! VDI Guideline 3783 Part 1 is limited to a max wind speed of 10 m/s, so that for DT1 only 10 m/s were used !!!!!!!!!!!!!

DT2: given wind speed 5,76 m/s in 2 m height results in 9,04 m/s in 10 m height using a power law with an exponent of 0,28

DT4: given wind speed 4,51 m/s in 2 m height results in 7,08 m/s in 10 m height using a power law with an exponent of 0,28

**Settings of Austal:**

Quality Paramter: 14

Computational Time: 600 s for Desert Tortoise and 1500s for FLADIS

Horizontal grid: minmum cell size 1 m x 1 m….grid growth: at 50 / 100 / 200 / 400 / 500 m distance by a factor of 2

Vertical grid: minimu cell height 0,2 m – within the 1st m over ground then growth bei 30% with each layer

Overall domain size: 1000 m length, 100 m height, 1000 m width for Desert Tortoise and 250 m length, 100 m height and 250 m width for FLADIS

Time step: 10 s

For all results the statistical uncertainty stayed below 10 %.