RESEARCH AND GUIDANCE FROM HSE

Effect of humidity on the dispersion behaviour of pressure-liquefied ammonia jet releases

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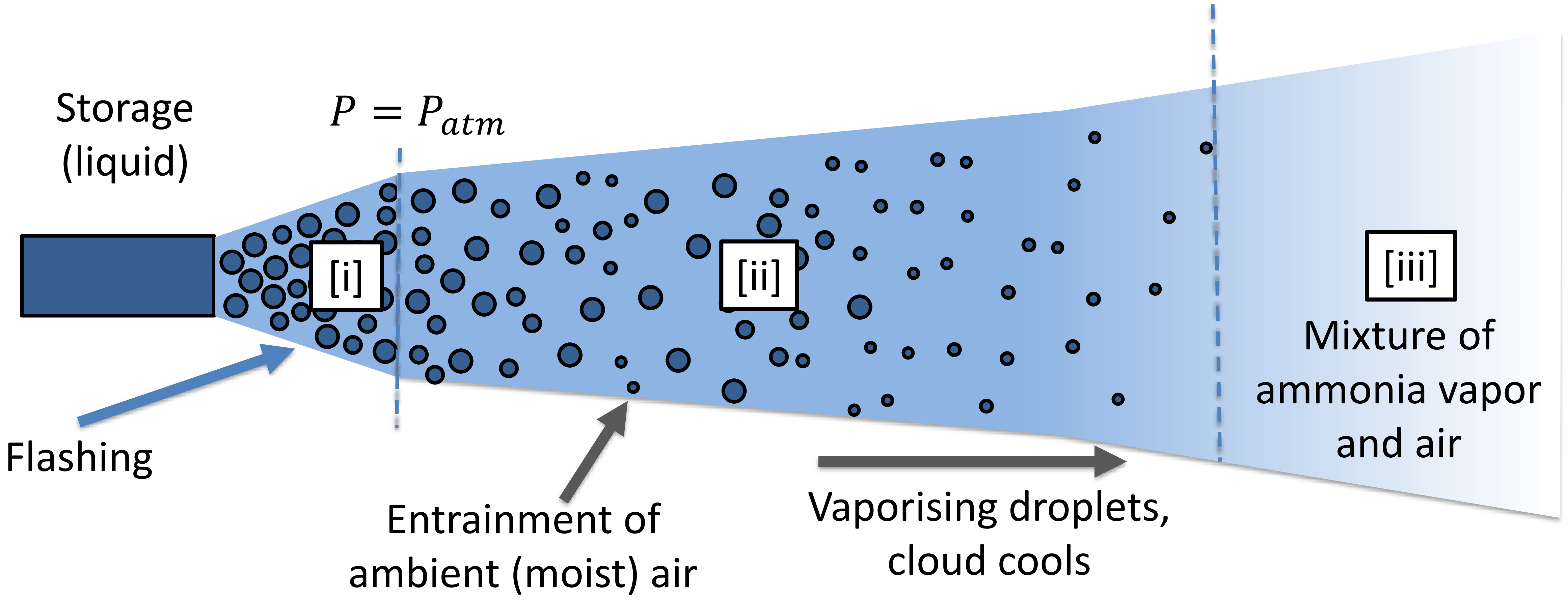
Contents

Pressure-liquefied ammonia jet release

What happens when pressure-liquified ammonia is released into the atmosphere?



- Region [i]
  - Flashing jet: rapid expansion, ammonia liquid partially flashes to vapor as pressure falls to ambient.
  - Temperature falls to ammonia boiling point at atmospheric pressure.
- Region [ii]
  - Air is entrained into the jet.
  - Ammonia droplets evaporate and cool the cloud temperature below the ammonia boiling point.
  - Humidity in the entrained air condenses as liquid water, releasing latent heat in the process.
  - Liquid droplets comprising a mixture of water and ammonia form a non-ideal solution, releasing heat of mixing.
  - Aqueous ammonia droplets evaporate as they are transported downstream in the jet: ammonia fraction decreases.
  - Cloud buoyancy relative to air depends on initial fraction of ammonia aerosol, ambient humidity and temperature.
- Region [iii]
  - All droplets have evaporated, cloud continues to entrain air and dilute.

Buoyancy of ammonia cloud- dry versus humid air

Haddock & Williams (1978) “The density of an ammonia cloud in the initial stages of atmospheric dispersion”, Safety and Reliability report SRD R 150, UK Atomic Energy Authority.

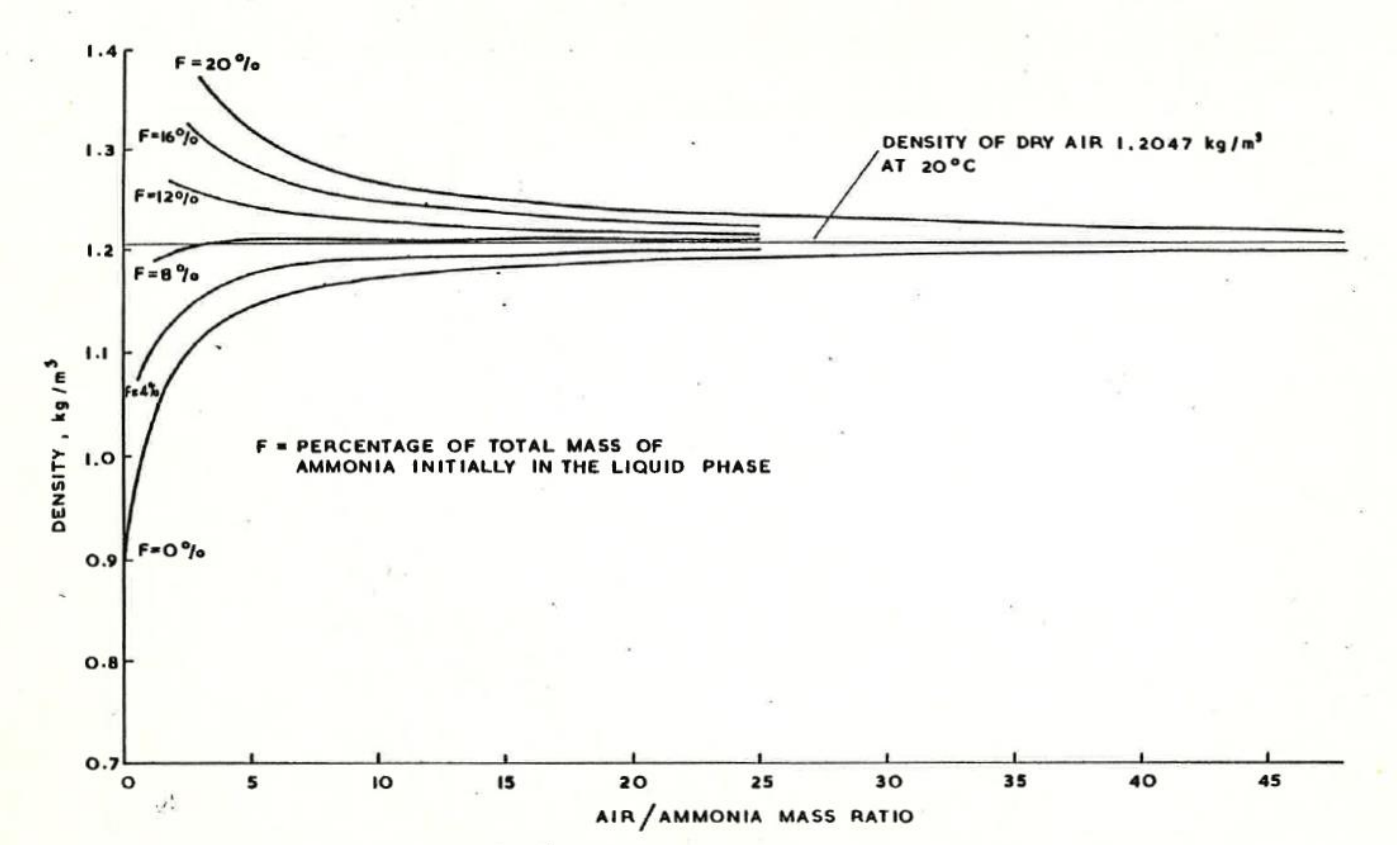


FIG. 6 DENSITY OF AN AMMONIA CLOUD INITIALLY CONTAINING SOME LIQUID AMMONIA AS IT IS DILUTED WITH DRY AIR

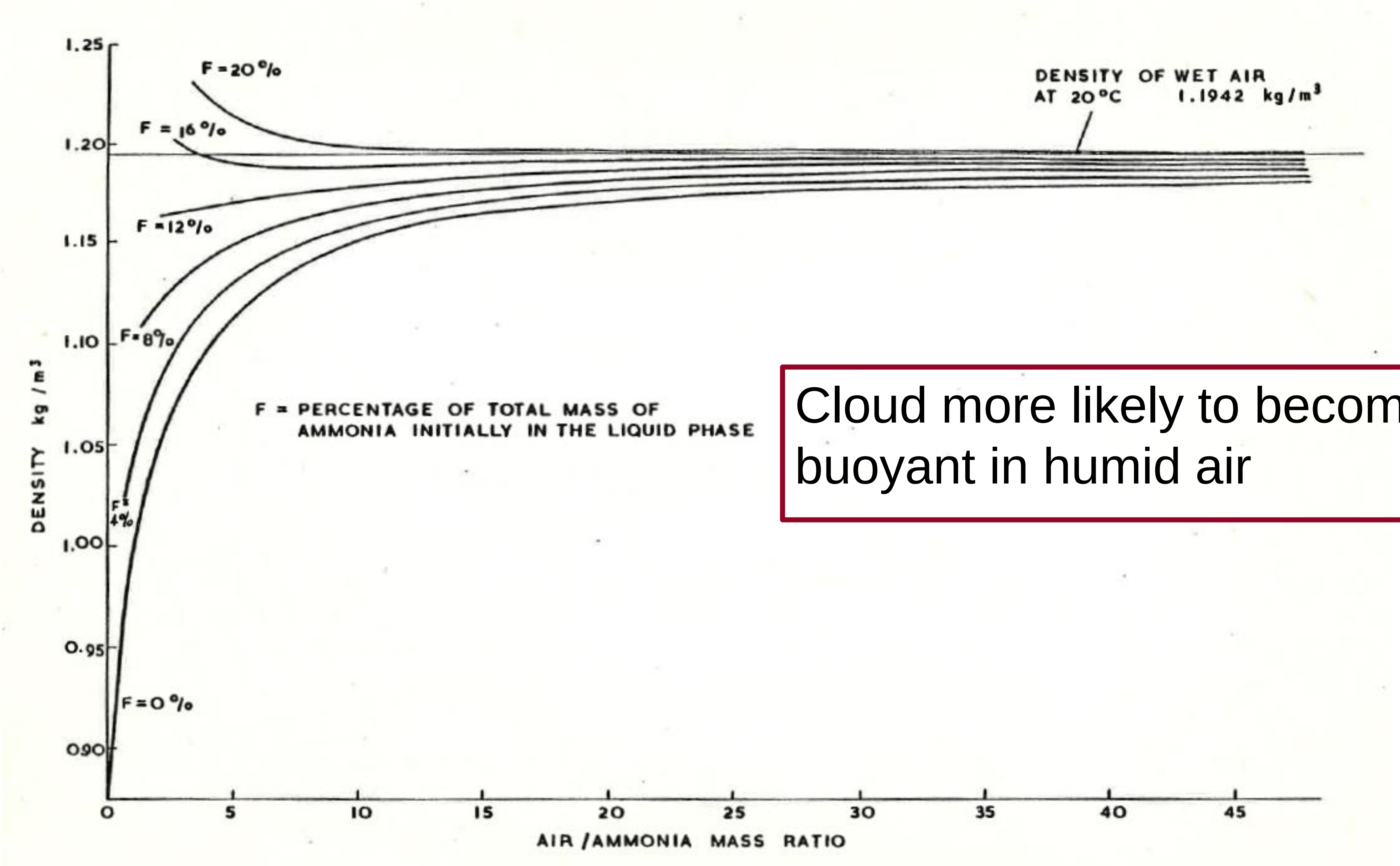


FIG. 8 DENSITY OF AN AMMONIA CLOUD INITIALLY CONTAINING SOME LIQUID AMMONIA AS IT IS DILUTED WITH WET AIR

Cloud more likely to become buoyant in humid air

DRIFT integral dispersion model

- DRIFT accounts for condensation of water from moist air into cold jet, mixing of liquid water droplets with ammonia droplets to form non-ideal aqueous ammonia solution, with associated thermodynamic effects.
- DRIFT v3.7.19 used.
- Each run typically takes < 1 min.
- Outputs examined here:
  - Arc-max concentration.
  - Cloud shape.

SRD R357

UNITED KINGDOM ATOMIC ENERGY AUTHORITY
SAFETY AND RELIABILITY DIRECTORATE

A theory of heterogeneous equilibrium between vapour and liquid phases of binary systems and formulae for the partial pressures of HF and H_2O vapour

by

C. J. Wheatley

SUMMARY

The thermodynamic basis of equilibrium systems composed of liquid and vapour phases of binary mixtures of miscible non-ideal substances is surveyed. This leads to the development of general formulae, for the saturated vapour pressures of the component substances, as functions of temperature and the liquid phase composition. The heat of mixing of the liquid phase and the properties of azeotropic mixtures are found. The formulae are studied in detail in the simplest non-ideal case and are successfully fitted to data for the HF-H_2O binary system. It is concluded that in this simplest case they have potentially wide applicability.

The work reported in this paper was carried out under contract for the Health and Safety Executive. The views expressed are those of the author and do not necessarily reflect the views or policy of the Health and Safety Executive.

April 1986 ISBN No: 0-85-356206-7

SRD R410

UNITED KINGDOM ATOMIC ENERGY AUTHORITY
SAFETY AND RELIABILITY DIRECTORATE

Discharge of liquid ammonia to moist atmospheres – survey of experimental data and model for estimating initial conditions for dispersion calculations

by

C. J. Wheatley

SUMMARY

A mathematical model is proposed for estimating concentrations near an accidental release of liquefied ammonia from a hole in a tank wall or from a severed pipe. Three quantities are particularly important for hazard assessment:

- the discharge rate;
- the fraction of liquid which rains out of the two-phase jet; and
- the amount of dilution with air up to a point where atmospheric mixing or gravitational effects become important.

As well as these, the model includes the chemical interaction of ammonia with atmospheric water vapour: this influences the mixture density and thus the rate of dilution in a subsequent heavy-gas dispersion phase.

Part I is a survey of relevant experimental data. In Part II, the mathematical details of the integral model are developed in sufficient detail for implementation in a computer code.

April 1987 ISBN No. 0-85-356220-2

Aims

Main purpose of work to answer question:

- How does humidity affect the dispersion behaviour of pressure-liquefied ammonia jet releases?

Further questions:

- Which release scenarios are most sensitive to humidity?
  - Does it depend on the ammonia release rate, ambient temperature and wind speed?
- For bounding cases, where humidity ranges from 0% to 100% RH, what are the differences in concentrations?

Methodology and Configuration of Simulations

- The Desert Tortoise field trials conducted in 1983 were selected as a suitable base test case.
- Conditions from Desert Tortoise Trial 1 were used, with the following changes:
  - Release duration was increased from 126 s to 10^4 s:
    - i.e., to simulate a continuous release.
  - Two release rates modelled:
    - 80 kg/s as in Desert Tortoise Trial 1.
    - 8 kg/s to assess impact of smaller release rate.
  - Wind speeds varied from 1.0 m/s to 5 m/s:
    - Desert Tortoise Trial 1 was 7.4 m/s.
  - Relative humidity varied from 0% to 100% RH.
  - Ambient temperature varied from 0°C to 30°C.
  - Neglect heat transfer from ground to cloud.

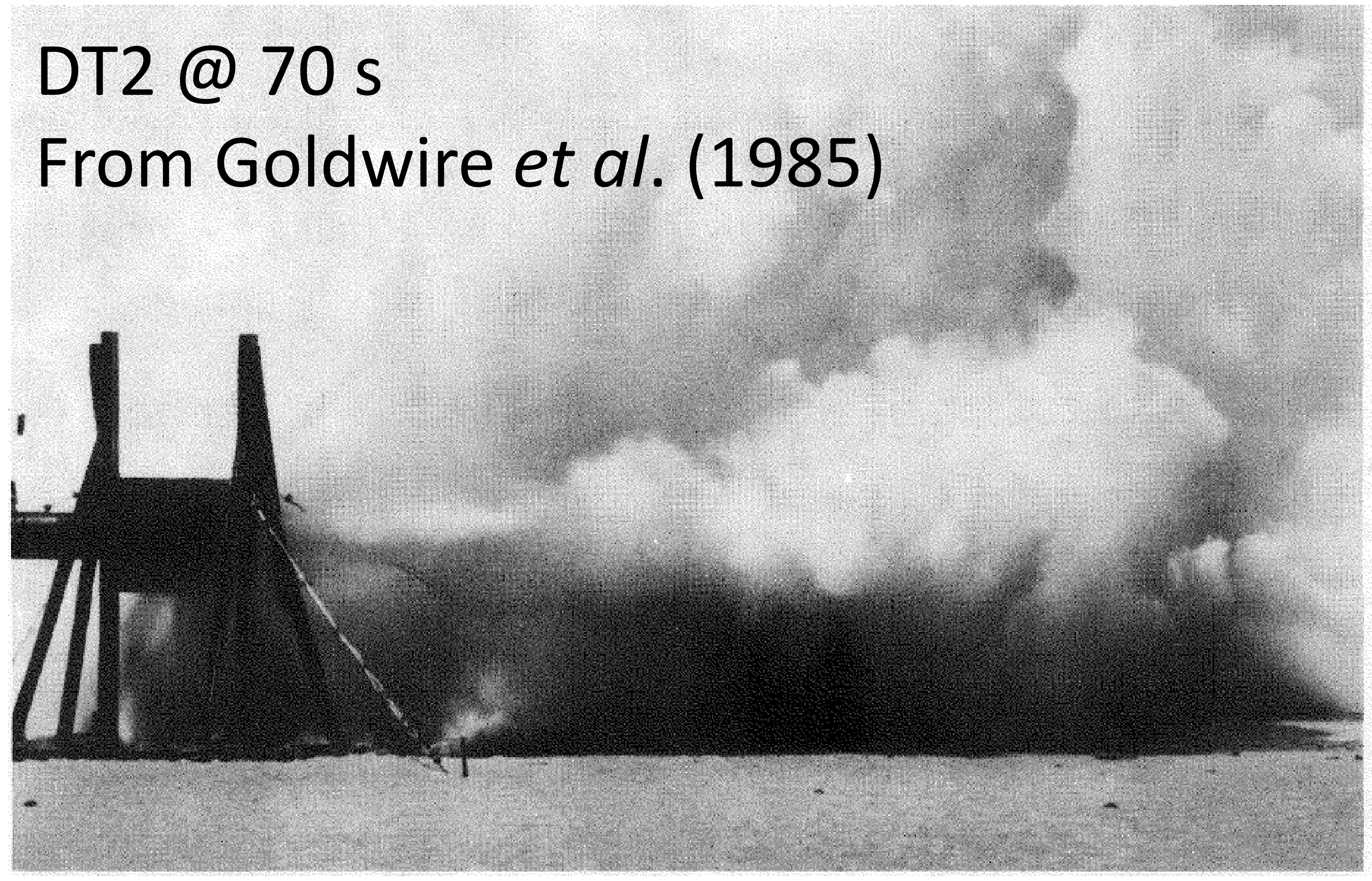
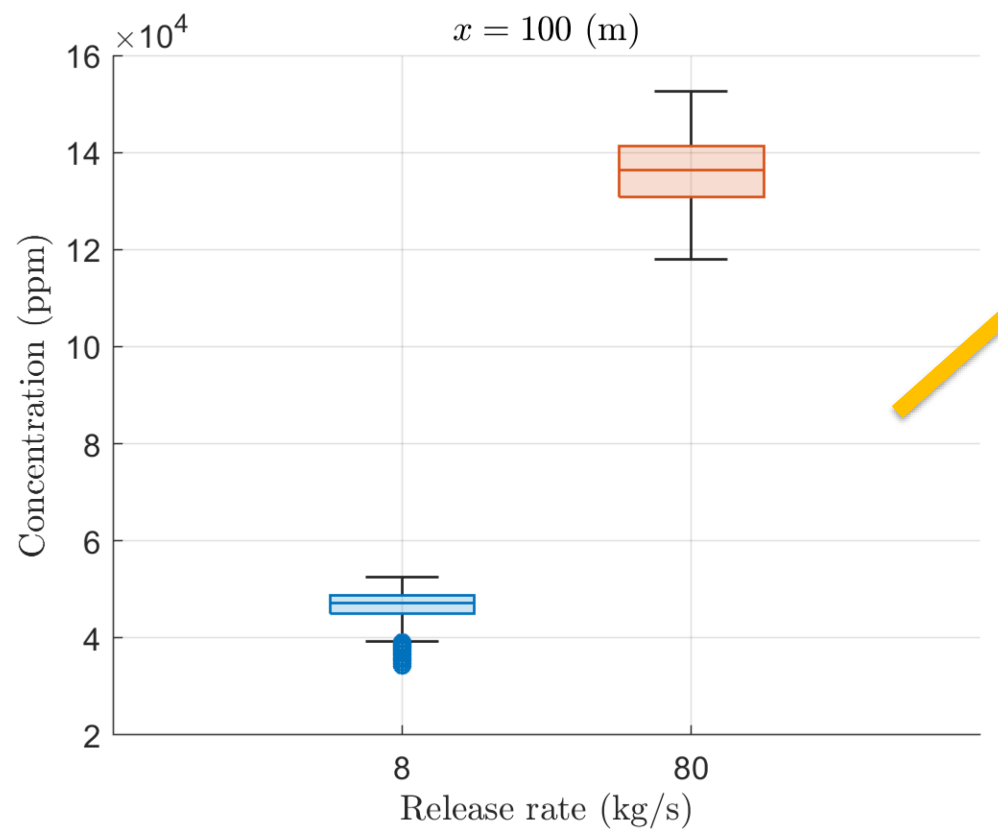
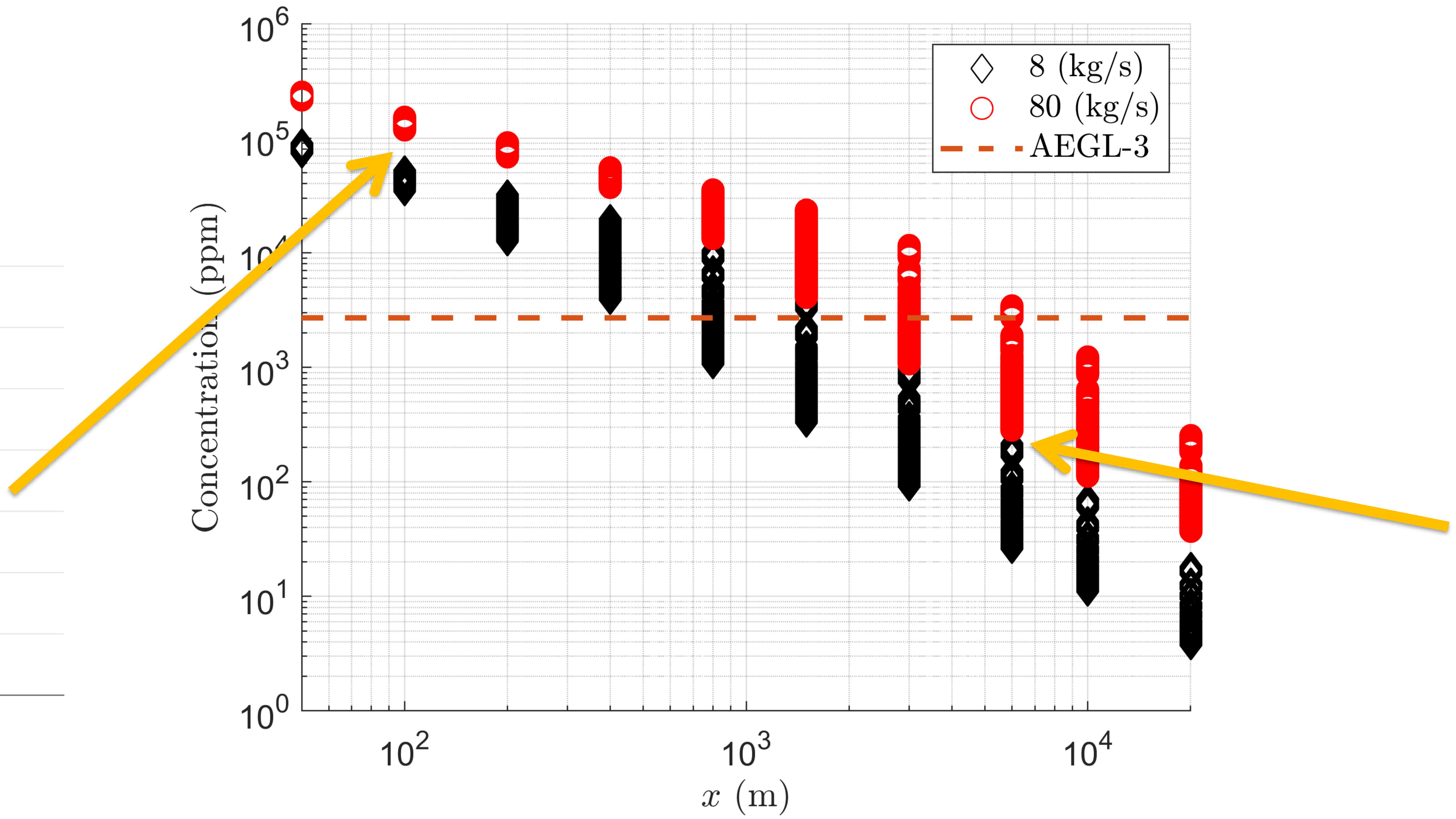


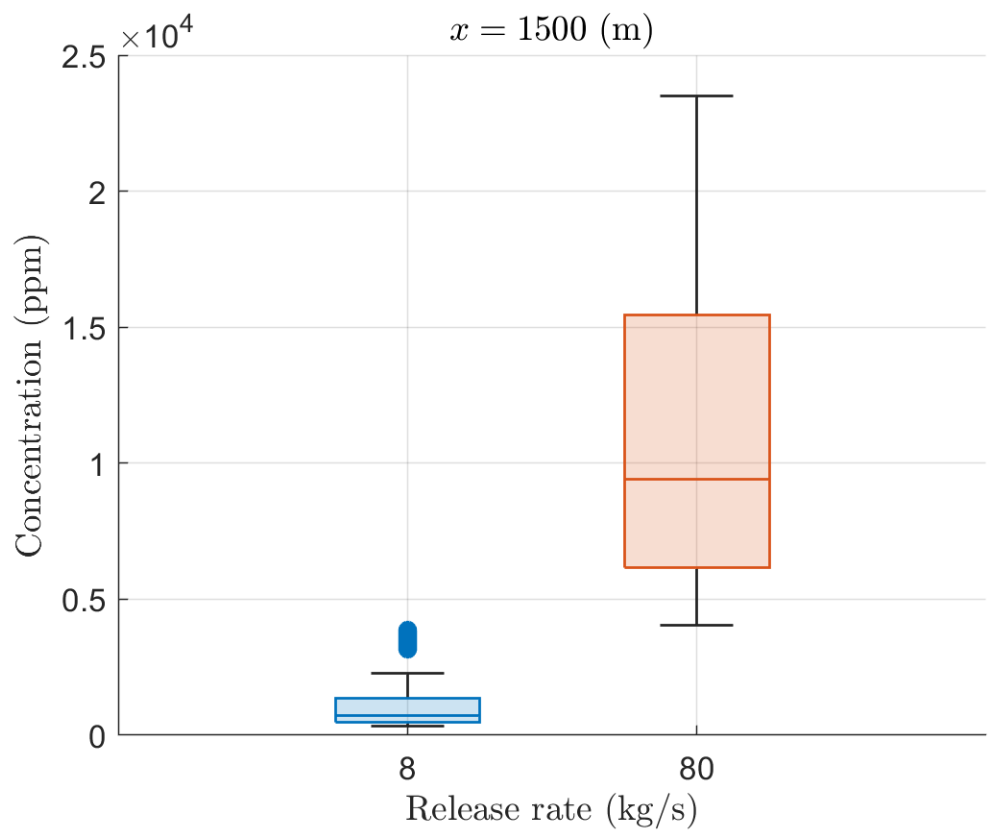
Fig. 15. Desert Tortoise 2 (upwind wide angle camera) Time = 230s. Lawrence Livermore National Laboratory

Centreline concentration

- Box charts consider the spread of concentration data.
- Large spread for 80 (kg/s) around 1500 (m).
- This corresponds to approximate distance to AEGL-3 (2700 ppm for 10 min exposure).
- The distance to AEGL-3 (x_{A3}) is an indicator of the downwind cloud extent.

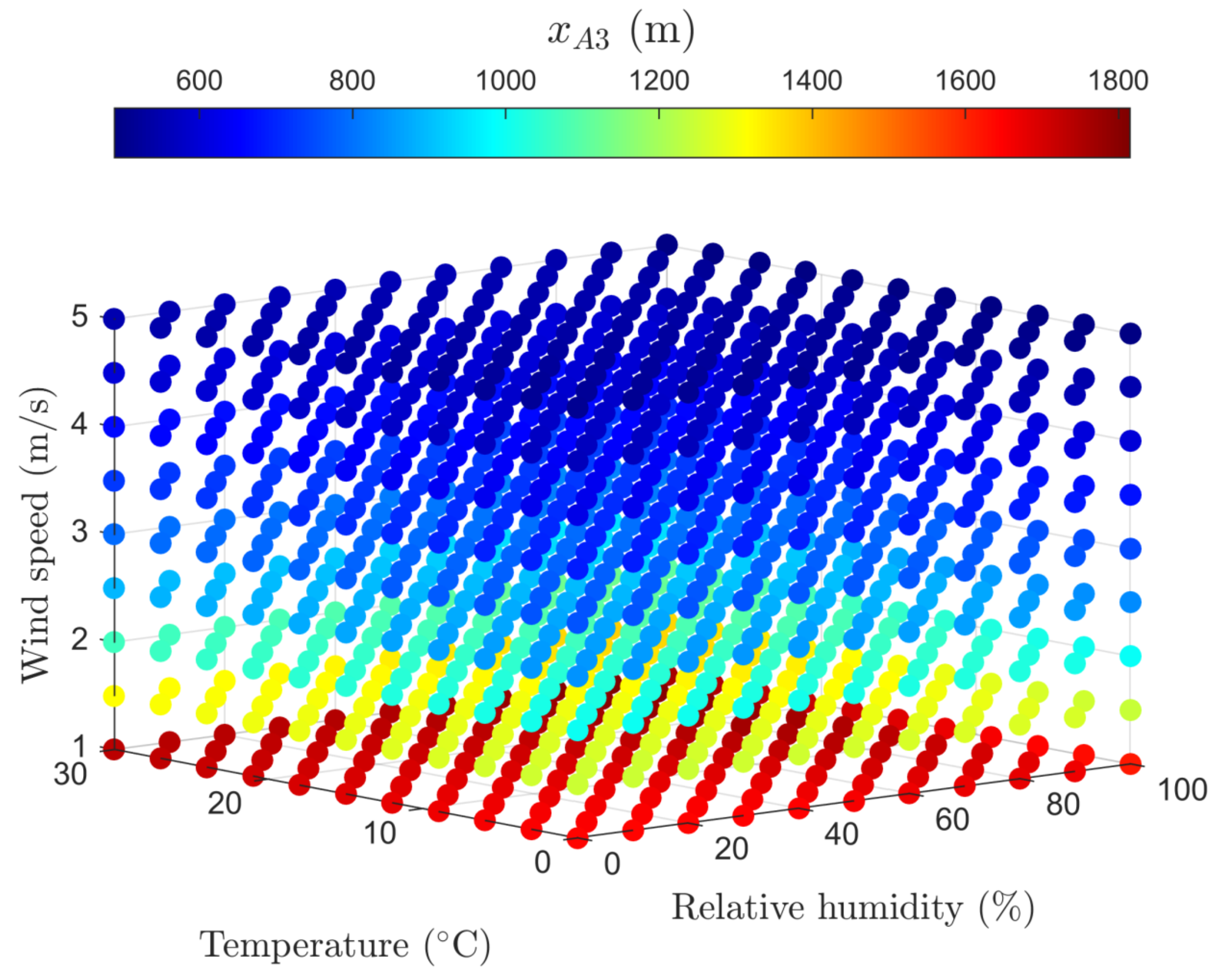




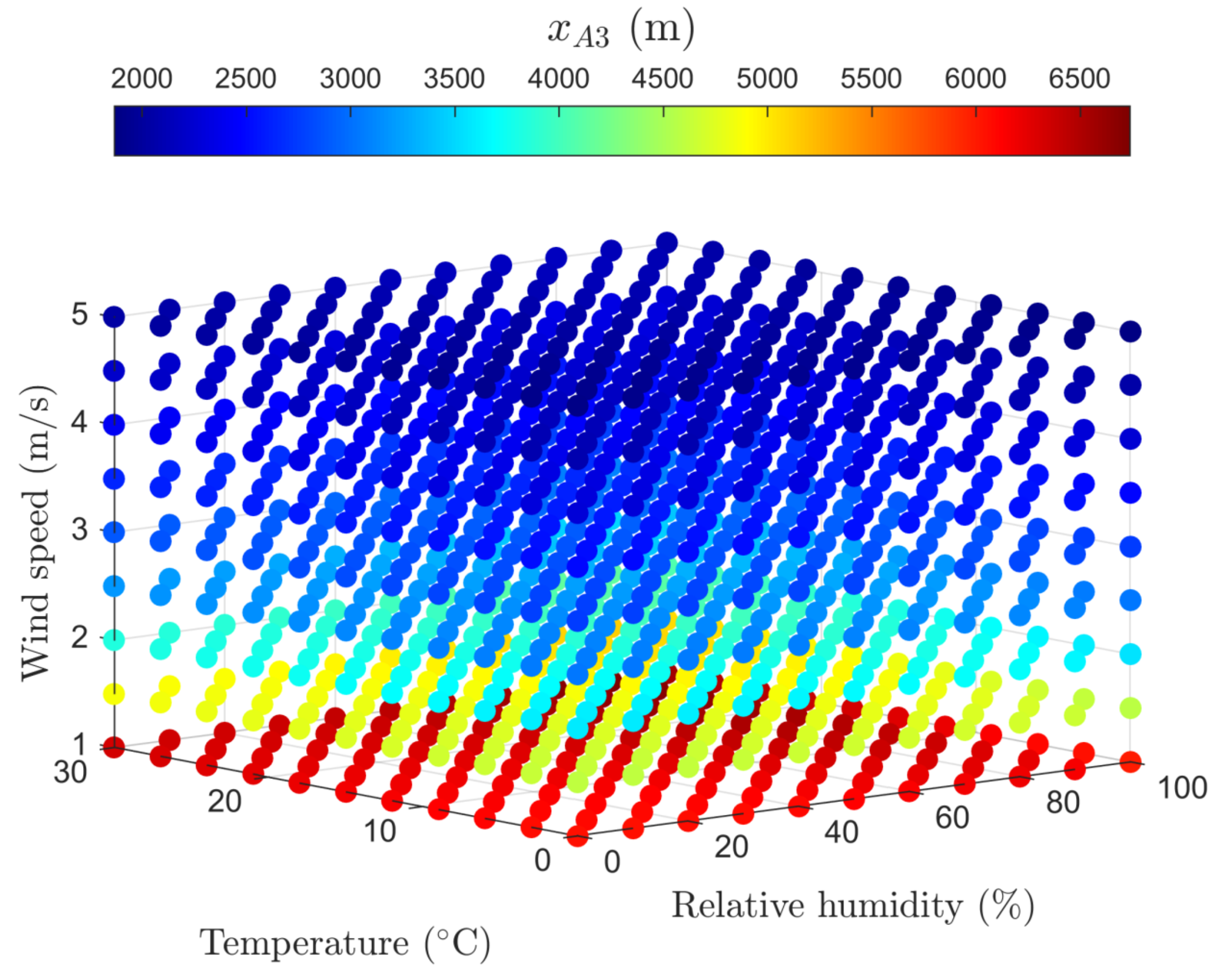


Wind speed and release rate

8 (kg/s)



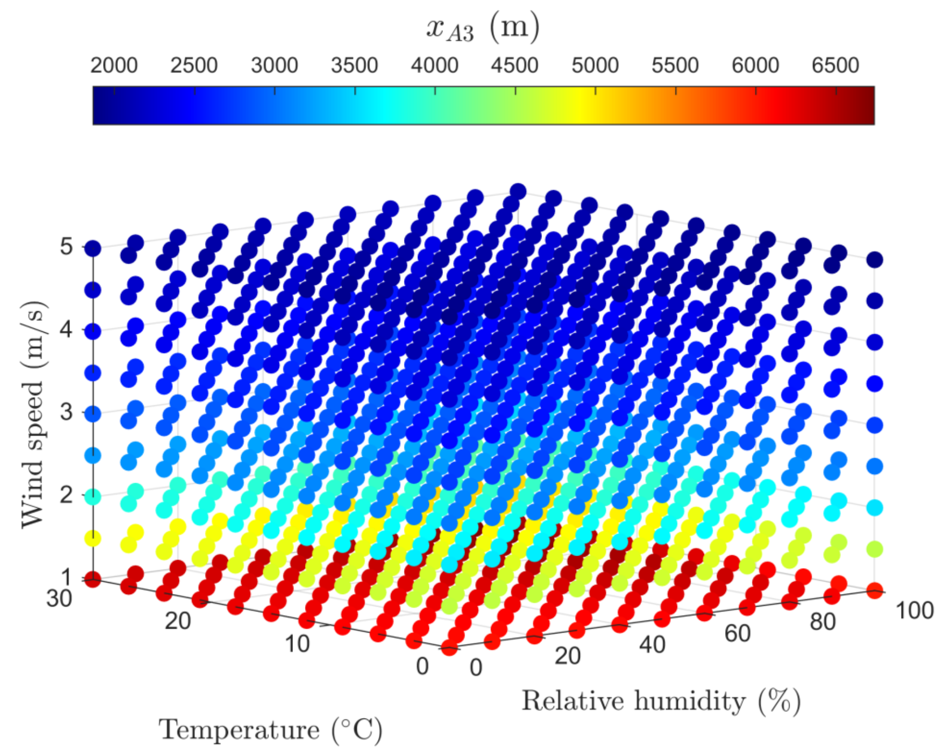
80 (kg/s)

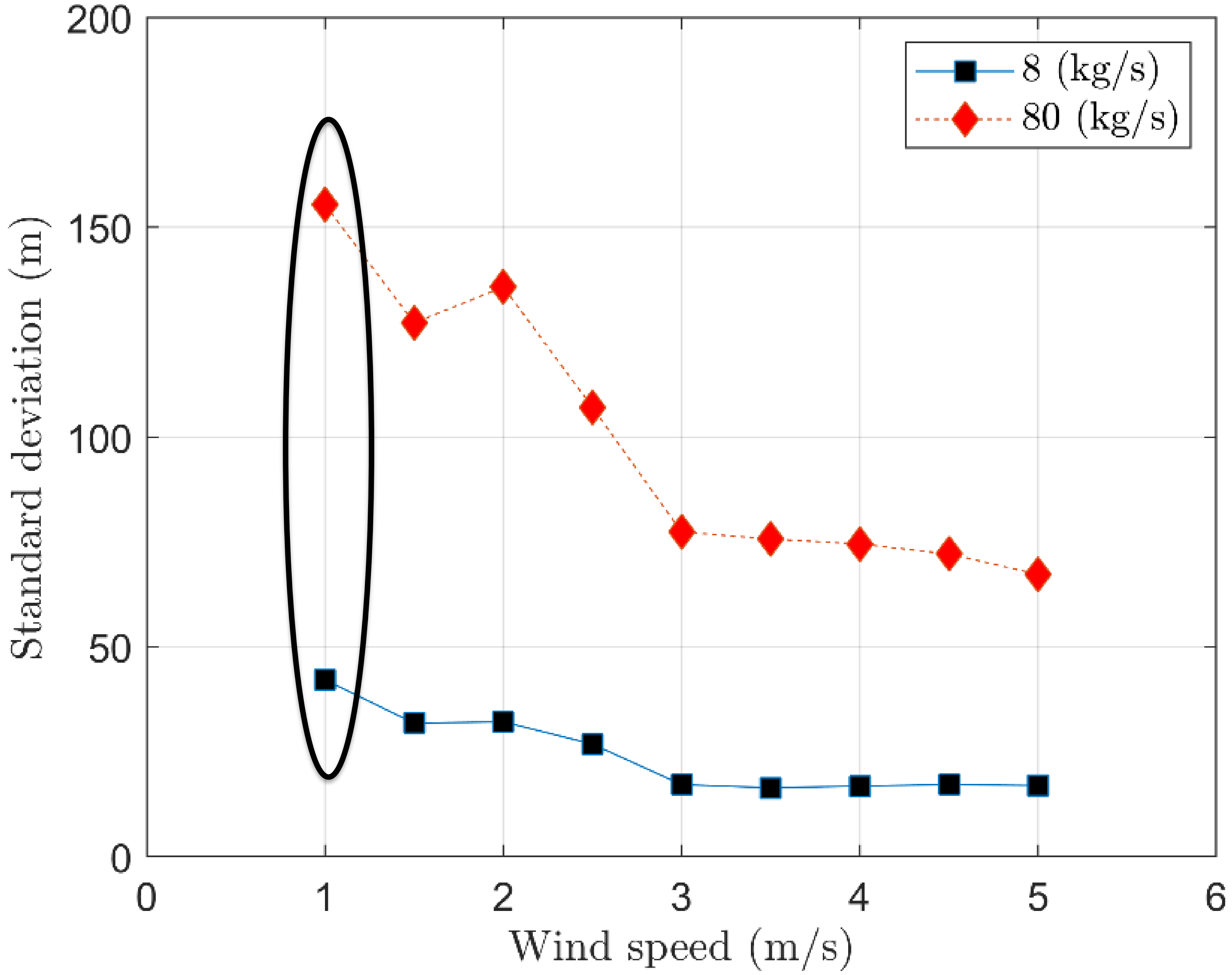


- Consider the distance to AEGL-3 (x_{A3}).
- Wind speed and release rate are the dominant factors affecting x_{A3}.
- This can be seen in the plots: colors are layered in the vertical direction (wind speed).
- Similar trends observed for the two release rates (although the absolute values of the distances x_{A3} are different, i.e., the scales of the colors).

Variance of results

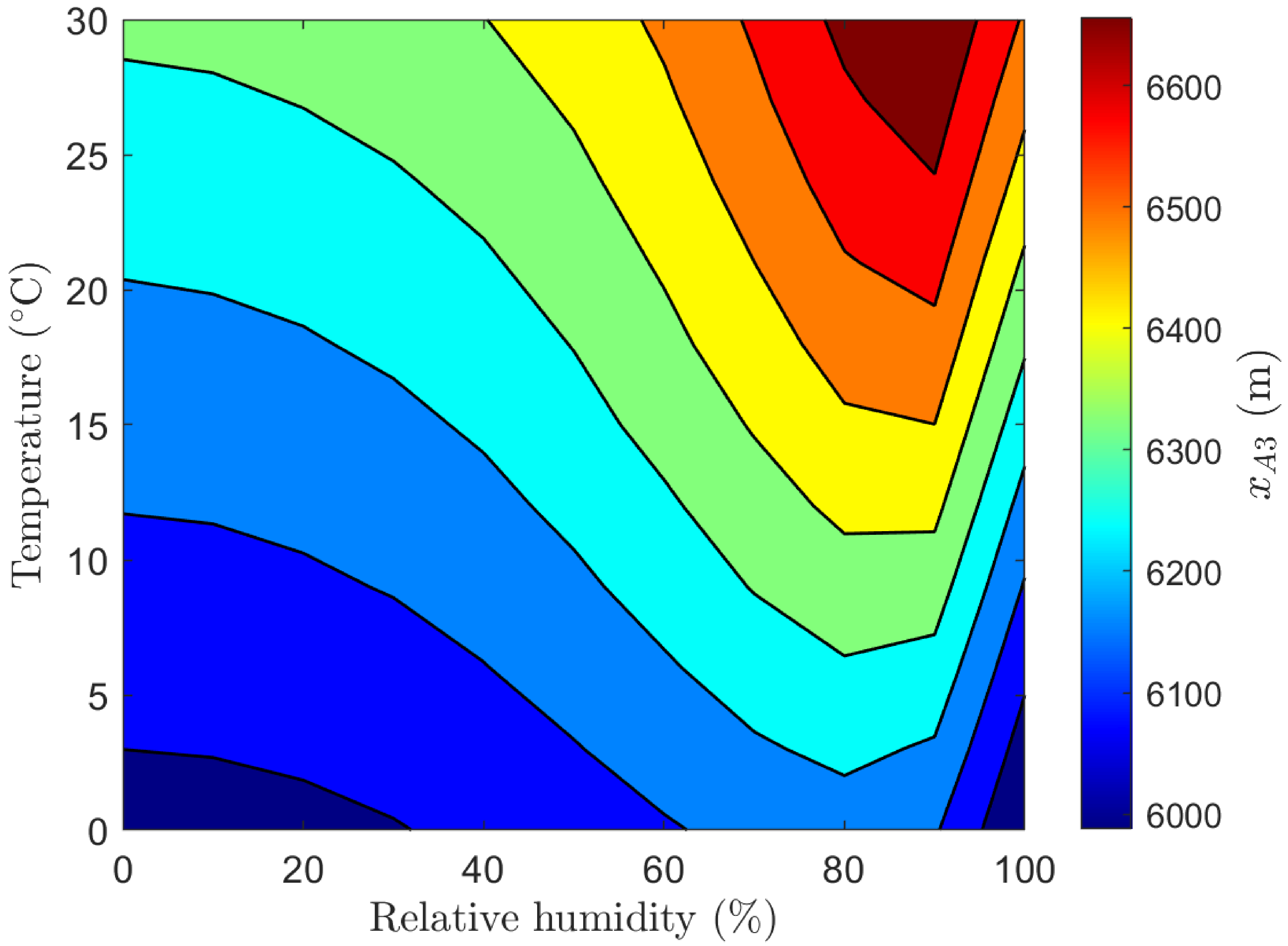
- For each horizontal layer, i.e., wind speed fixed, calculate the standard deviation from varying temperature and humidity.
- Greatest variance at low wind speeds and high release rate.
- Standard deviation (generally) decreases as the wind speed increases.
- **We focus next on the most sensitive case:**
  - **lowest wind speed of 1 m/s.**
  - **highest release rate of 80 kg/s.**





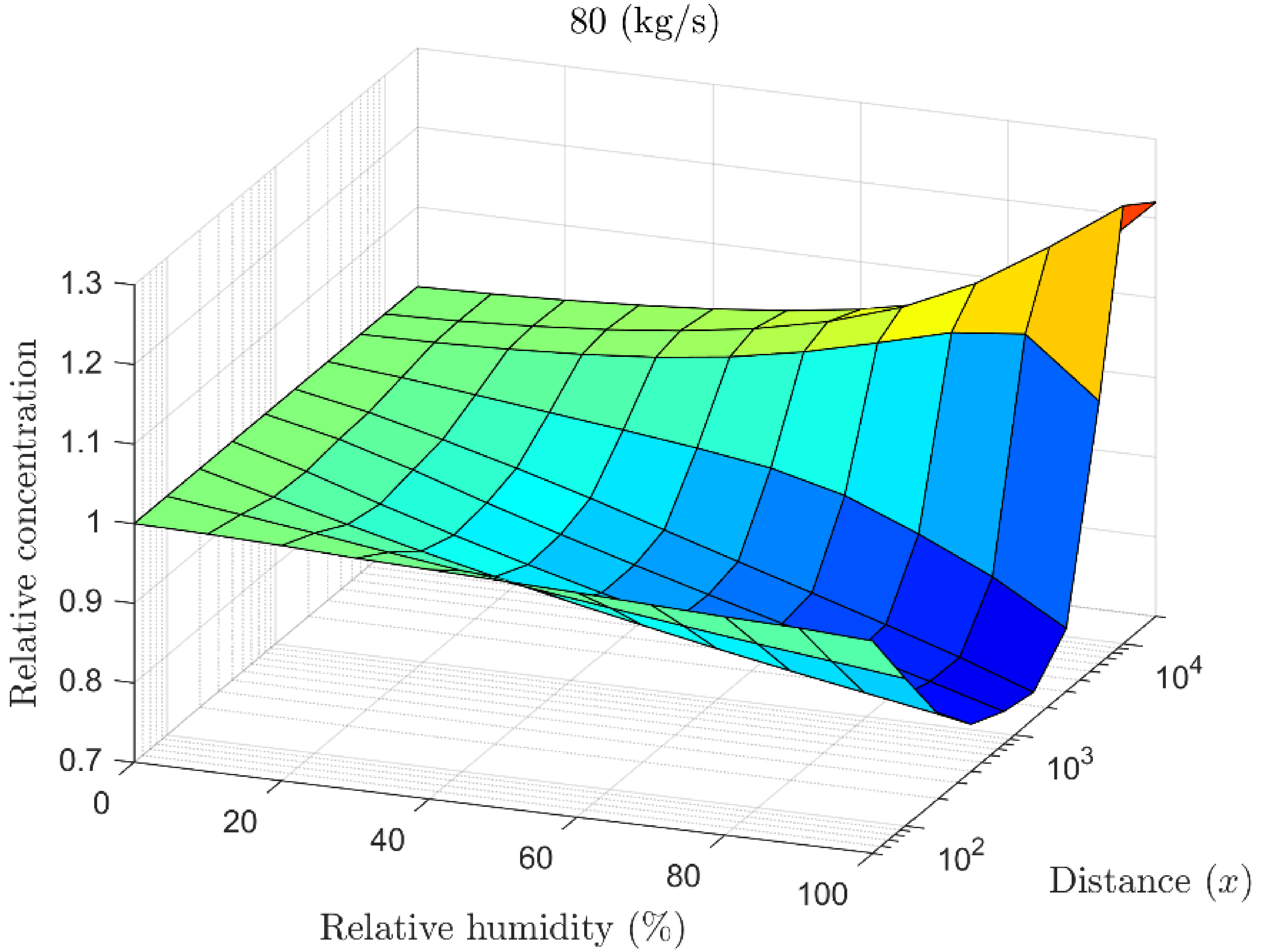
Temperature versus humidity

- Increasing the temperature (for a fixed humidity) results in a larger distance to AEGL-3:
  - Moving vertically upwards in the plot, x_{A3} always increases.
- Increasing humidity from 0% to 80% RH (temperature fixed) results in an increase in x_{A3}.
- However, increasing humidity further from 80% to 100% results in a reduction in x_{A3}.
- Largest values of x_{A3} found at maximum temperature of 30 °C and a humidity of ≈ 90% RH.



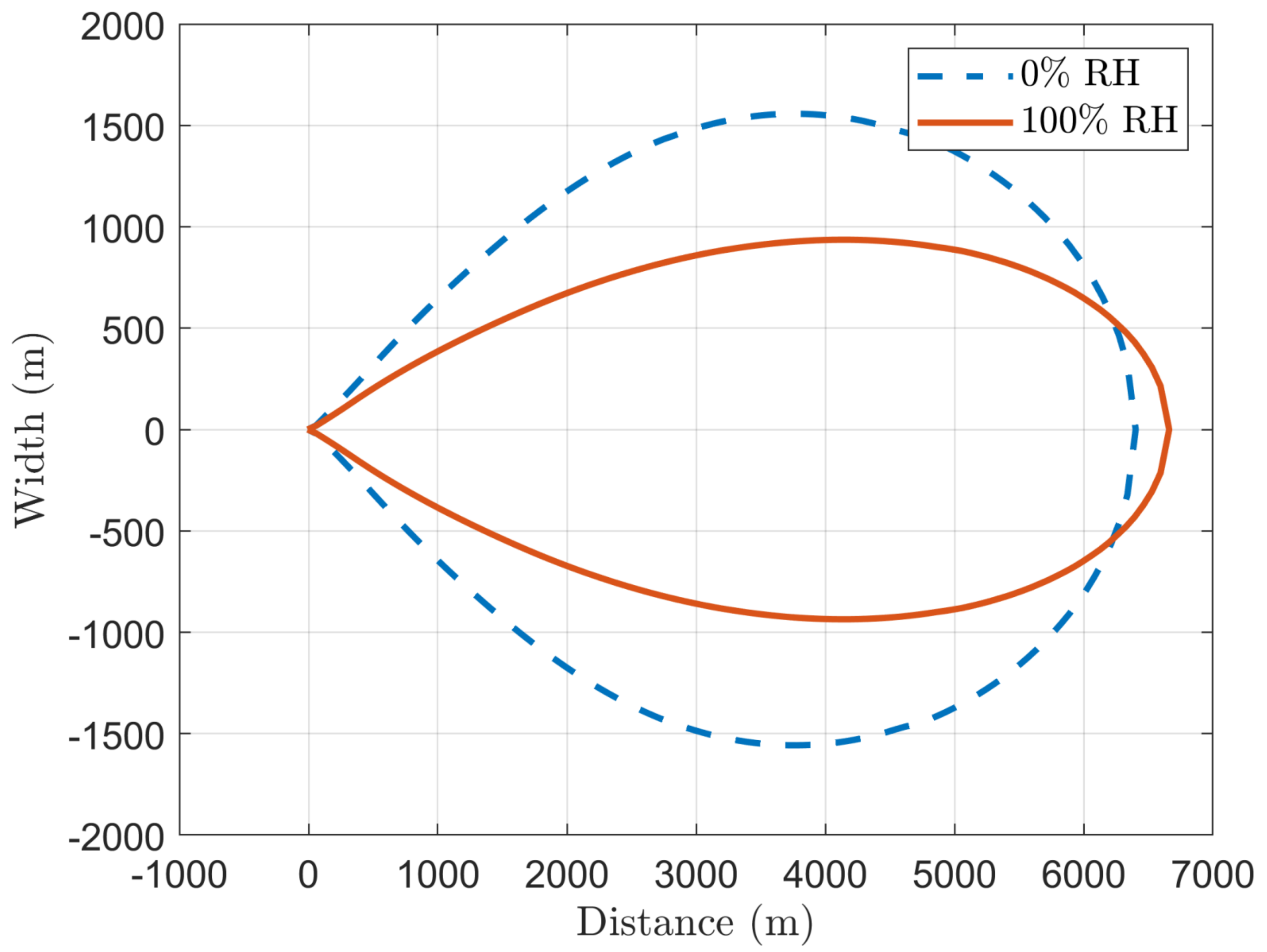
Relative concentration with distance

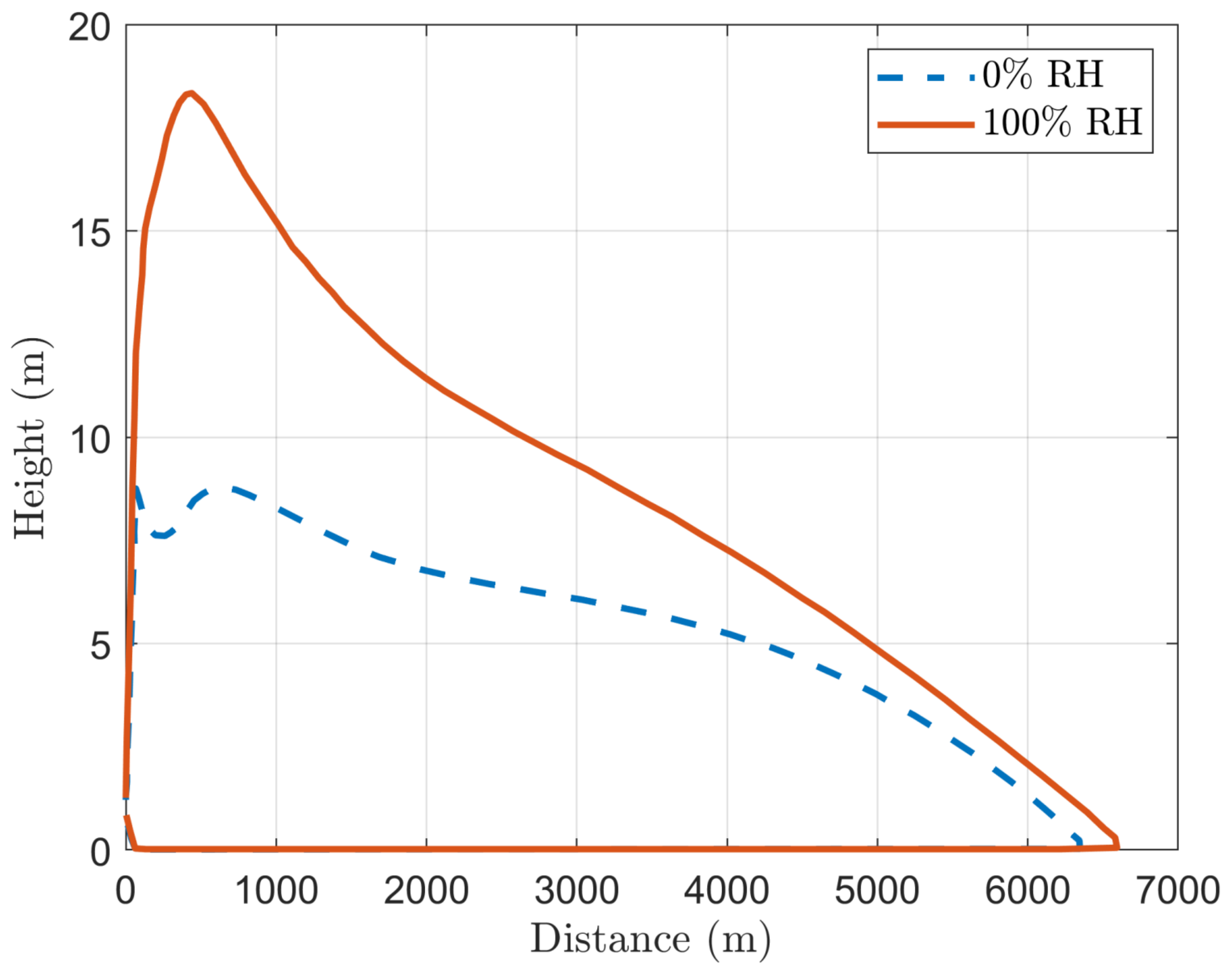
- Surface plot of predicted concentration relative to the completely dry (0% RH) concentration.
- Fixed temperature of 30 °C.
- Concentrations are within ±30% of the results for a completely dry atmosphere.
- What is causing the complex behaviour?
  - Ideal versus non-ideal ammonia solution?
  - Density of moist air relative to dry air?



Shape of clouds

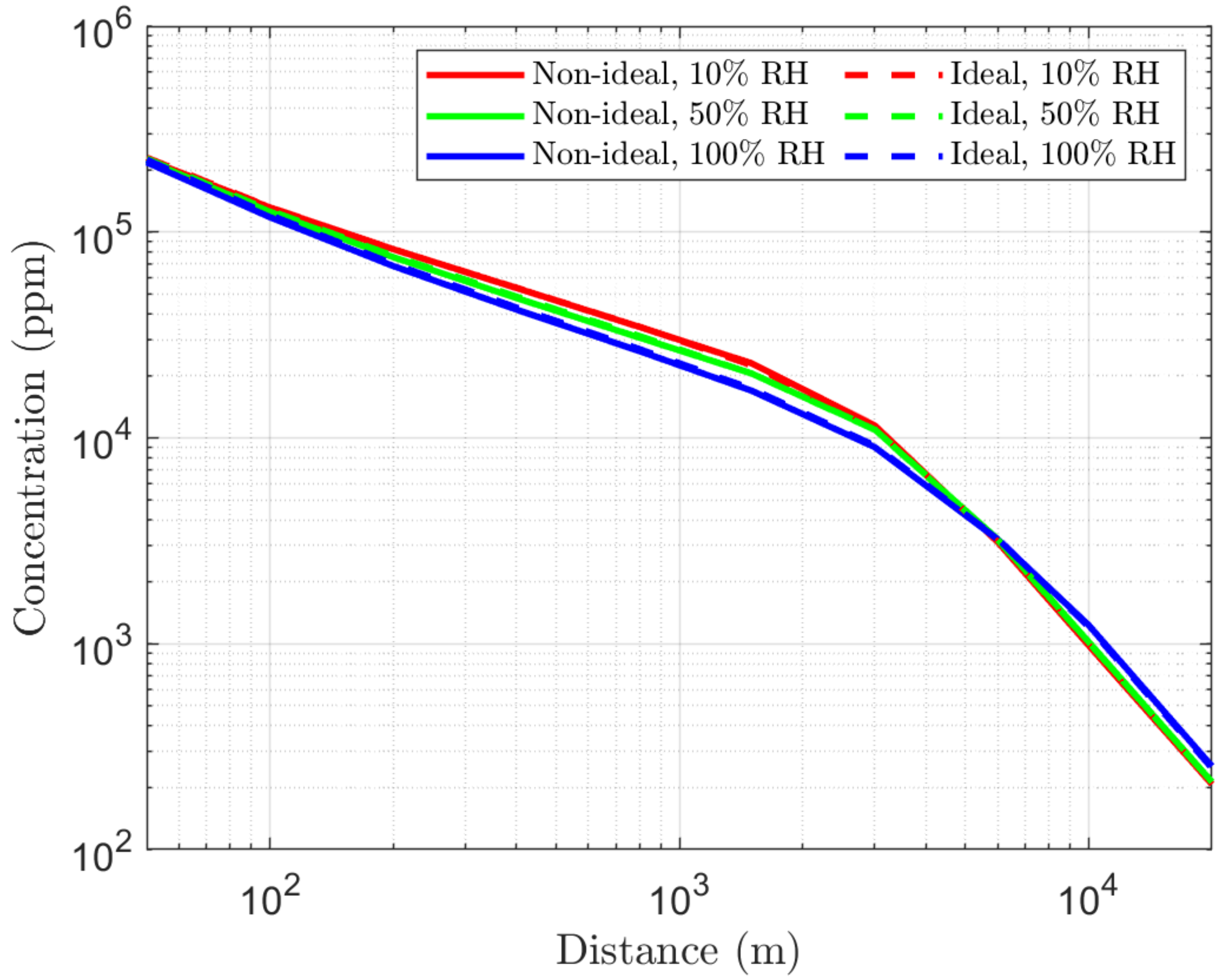
- Cloud shape, namely width and height, is plotted for contours of AEGL-3 (2700 ppm).
- Cloud width is reported at a height of 1 m.
- Increasing the relative humidity from 0% to 100% alters the shape of the cloud:
  - The cloud becomes narrower, but taller.

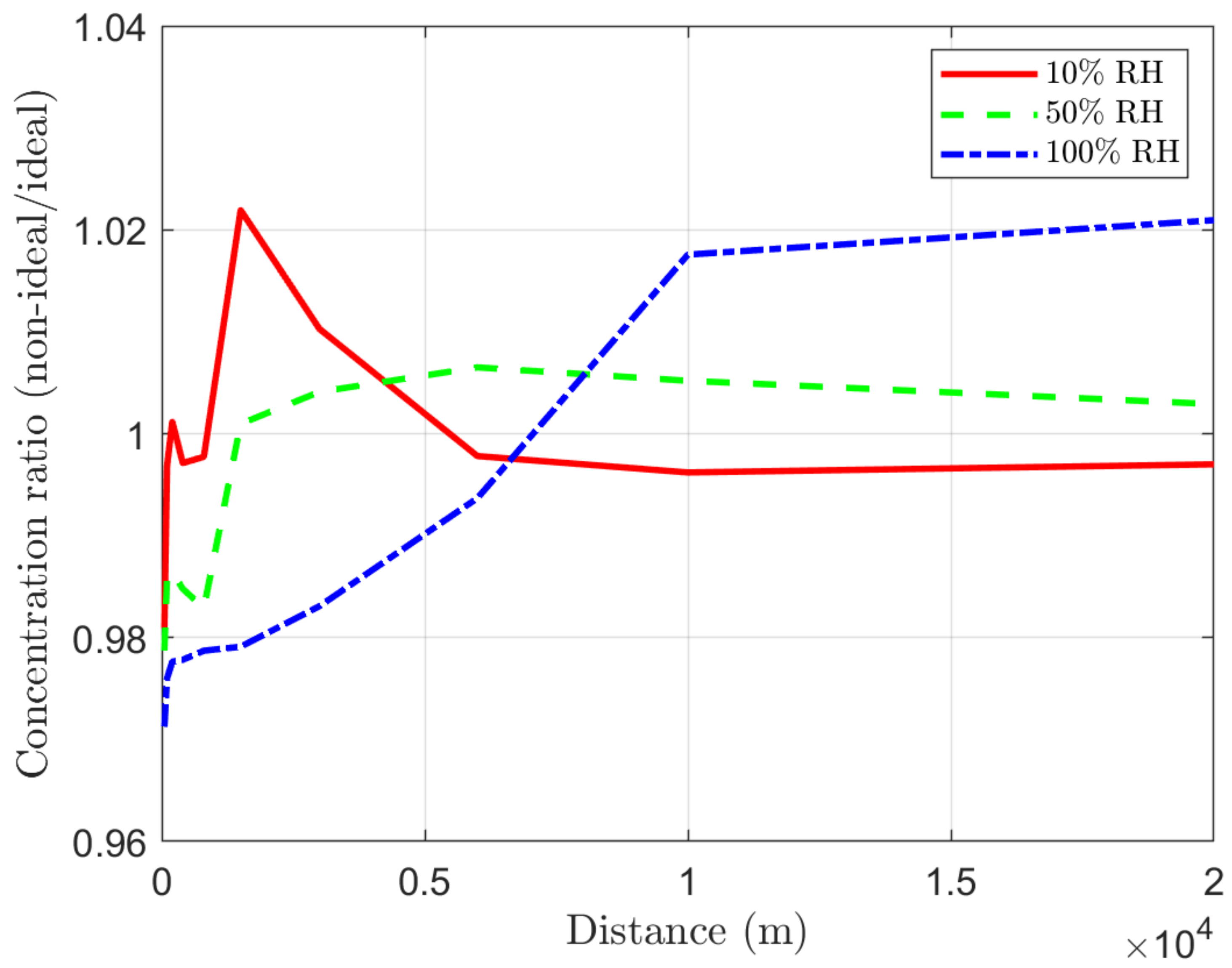




Ideal solution versus non-ideal solution

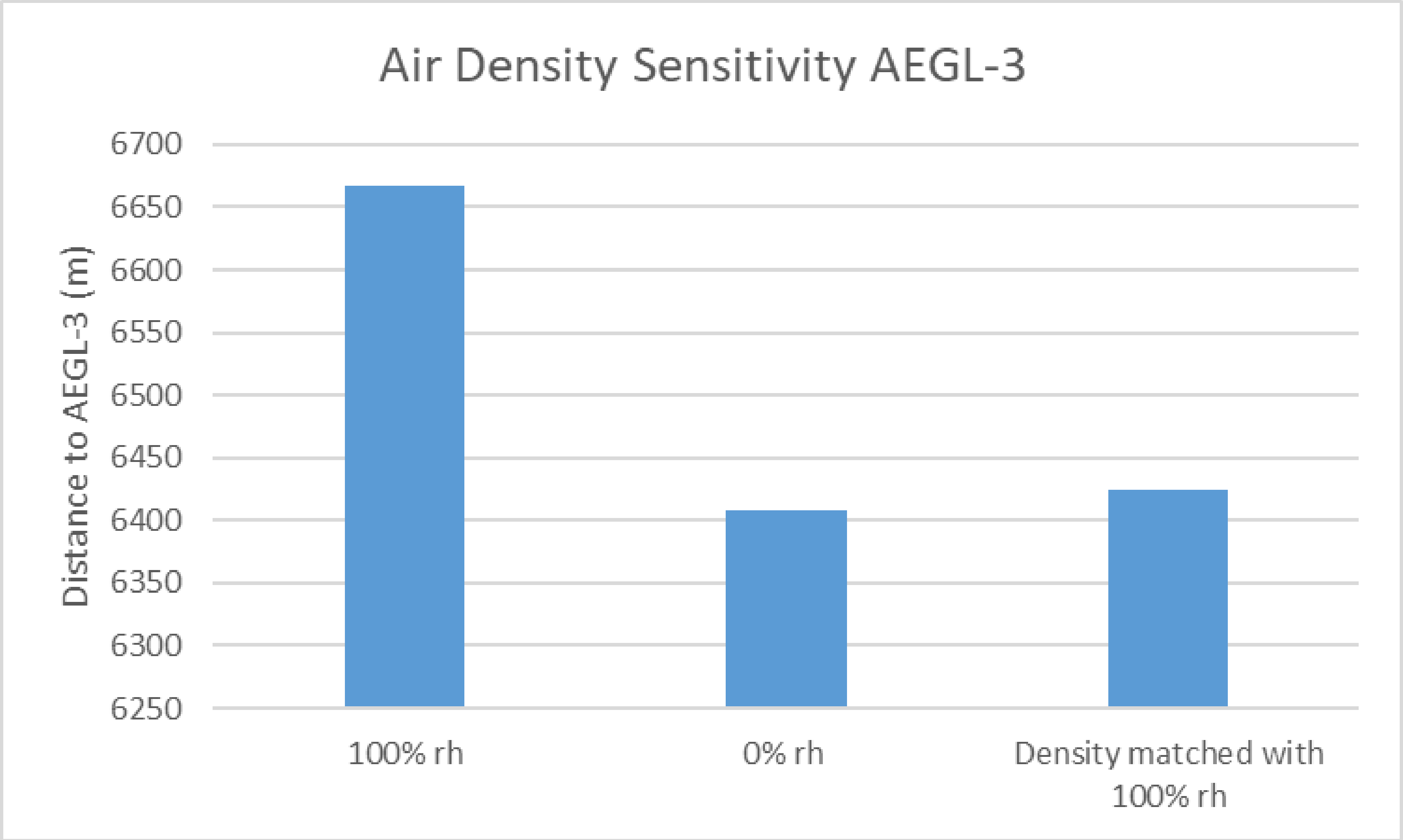
- Simulations were also run with an **ideal solution** sub-model which has no heat of mixing.
- The ideal and non-ideal solution results are within ±3%.
- Therefore, although ammonia and water form a non-ideal solution, this does not account for the ±30% effect seen in the earlier slide.





Air density versus thermodynamics

- Is the observed behaviour with humidity simply due to the change in air density or is it a thermodynamic effect?
- Compare predicted distance to AEGL-3 for dispersion in:
  - 100% relative humidity.
  - 0% relative humidity.
  - A dry ambient fluid with density matched (by adjusting molecular weight) to moist air at 100% relative humidity.
- Results indicate:
  - The density matched to 100% humid air case is closer to the 0% relative humidity case than the 100% humidity case.
  - The behaviour with relative humidity appears to be dominated by thermodynamics (water condensation and evaporation) rather than ambient density.



Conclusions

- When is the ammonia dispersion behaviour most sensitive to humidity?
  - Greatest sensitivity is observed for the highest release rate, lowest wind speed and highest air temperature cases.
- How does humidity affect the dispersion?
  - The overall predicted effect on concentrations is generally small (less than ±30% change) .
  - Complex behaviour is observed where humidity increase can either increase or decrease predicted concentrations depending upon distance from the source.
  - Increasing air temperature produces a small increase predicted concentrations.
  - In the most sensitive case, the distance to the AEGL-3 harm criteria increased by approximately 10% when the humidity increased from 0% RH to 80% RH and then decreased at higher humidity.
  - In comparison, increasing the wind speed from 1 m/s to 5 m/s decreased the distance to AEGL-3 by a factor of three.
  - Buoyant lift off was not predicted for any of the cases simulated here, although the depth of the cloud increased when the atmosphere was more humid.
- Although ammonia forms a non-ideal solution with water, which has been modelled, an ideal solution model with no heat of mixing was found to behave similarly (the predicted distances to AEGL-3 were within ±3% of the non-ideal).
- The dominant influence appears to be due to the condensation and evaporation of water (and associated latent heat effects) within the cloud, rather than simply due to the density of air changing with humidity.

Further work

- A low-momentum source might show greater effects of humidity.
  - We could potentially repeat the exercise for an instantaneous (puff) release?
- Non-pressure liquefied ammonia spill scenarios may also exhibit different sensitivities due to:
  - Reduced or no entrainment of ammonia liquid directly from the source into the cloud compared with pressure liquefied releases.
  - Potential for condensation of ammonia vapor above a cold pool source.
  - Possible dense gas blanket formation over pool.
  - Greater potential for forming buoyant clouds.

Thank you

Any questions?

- Contact: simon.gant@hse.gov.uk
- The contents of this presentation, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy

Appendix A- Heat transfer from ground