

# **Dense gas dispersion**

**An introduction from the perspective of HSE Science Division**

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Presentation to Atmospheric Dispersion and Air Quality (ADAQ) group, Met Office, UK

18 April 2024

**Research** - HSE funded to provide evidence which underpins its policy and regulatory activities

**Guidance** - freely available to help people comply with health and safety law

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- Introduction to HSE
- Dense gas dispersion physics
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**Acknowledgment:** this work draws heavily on the review by Rachel Batt (2021) for the Atmospheric Dispersion Modelling Liaison Committee [www.admlc.com/publications](http://www.admlc.com/publications)

# Introduction to HSE

- HSE is the UK regulator for workplace health and safety
  - Includes onshore/offshore pipelines, chemical/oil/gas infrastructure, offshore platforms etc.
  - Activities: evidence gathering, policy development, consultation, regulation, incident investigation, enforcement
  - HSE acts as an enabling regulator, supporting the introduction of new technologies
  - 2,400 total staff
  - £230M (\$280M) budget: 60% from the Government, 40% from external income

- HSE Science and Research Centre, Buxton, UK
  - 400 staff, 550-acre test site
  - Scientific support to HSE and other Government departments
  - “Shared research” or joint-industry projects co-funded by HSE
  - Bespoke consultancy on a commercial basis



# Dense gas dispersion physics

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- Flow generated by density differences
- Plume spreads with increased horizontal and reduced vertical extent (as compared to a passive plume)
- Profiles of concentration in lateral direction are often quite uniform
- Little meandering of plume due to random environmental flow
- Shear between plume and environment induces mixing
- Stably-stratified conditions reduce turbulence
- Inertia of the cloud depends on the density of the released material



# Why is HSE interested in dense gas dispersion?



Jack Rabbit II Trial 8 chlorine release © DHS S&T CSAC <https://www.uvu.edu/es/jack-rabbit/>

- Dense gases often fall to the ground, even if they are released from height
- Dispersing clouds of dense gas, spreading along the ground can lead to:
  - High concentrations of toxic gases in our breathing zones
  - Increased chances of flammable clouds reaching ignition sources
- Many of the toxic and flammable substances of interest to HSE produce dense gases

# Substances of interest to HSE

## Control of Major Accident Hazards (COMAH) regulations

Column 1	CAS number (1)	Column 2	Column 3
Dangerous substances		Qualifying quantity in tonnes of dangerous substances for the application of:	
		Lower tier requirements	Upper tier requirements
35. Anhydrous ammonia	7664-41-7	50	200
36. Boron trifluoride	7637-07-2	5	20
37. Hydrogen sulphide	7783-06-4	5	20
38. Piperidine	110-89-4	50	200
39. Bis(2-dimethylaminoethyl) (methyl)amine	3030-47-5	50	200
40. 3-(2-Ethylhexyloxy)propylamine	5397-31-9	50	200
41. Mixtures of sodium hypochlorite classified as Aquatic Acute Category 1 [H400] containing less than 5 % active chlorine and not classified under any of the other hazard categories in Part 1 of this Schedule, provided that the mixture in the absence of sodium hypochlorite would not be classified as Aquatic Acute Category 1 [H400]	-	200	500
42. Propylamine (see note 21)	107-10-8	500	2,000
43. Tert-butyl acrylate (see note 21)	1663-39-4	200	500
44. 2-Methyl-3-butenitrile (see note 21)	16529-56-9	500	2,000
45. Tetrahydro-3,5-dimethyl-1,3,5-thiadiazine-2-thione (Dazomet) (see note 21)	533-74-4	100	200

Etc. <https://www.hse.gov.uk/pubns/priced/l111.pdf>

## Planning (Hazardous Substances) Regulations

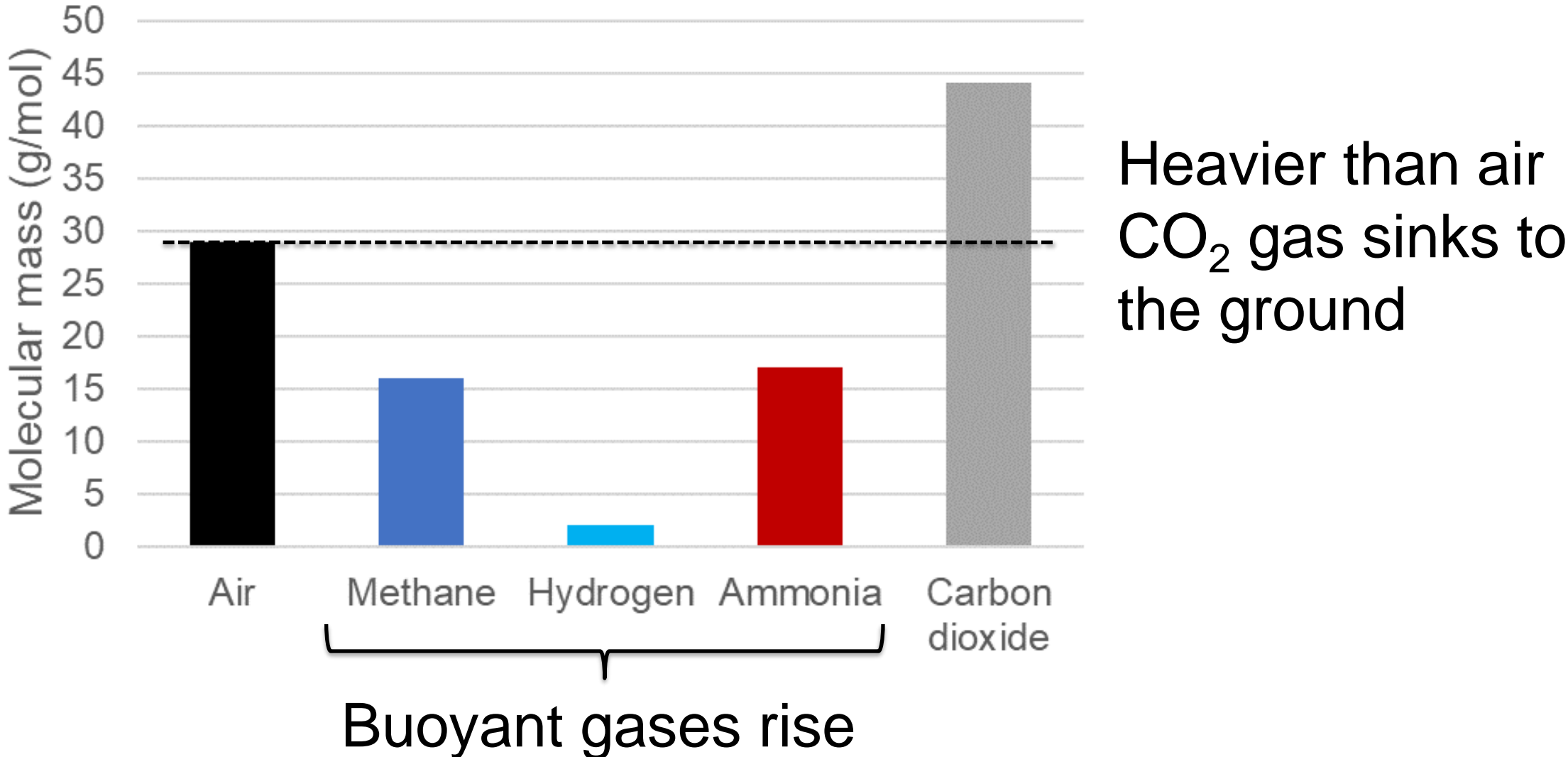
Named hazardous substances		
Column 1	CAS number <sup>(1)</sup>	Column 2
Hazardous substances		Controlled quantity (tonnes)
1. Ammonium nitrate (see note 14)	-	5,000
2. Ammonium nitrate (see note 15)	-	1,250
3. Ammonium nitrate (see note 16)	-	350
4. Ammonium nitrate (see note 17)	-	10
5. Potassium nitrate (see note 18)	-	5,000
6. Potassium nitrate (see note 19)	-	1,250
7. Arsenic pentoxide, arsenic (V) acid and/or salts	1303-28-2	1
8. Arsenic trioxide, arsenious (III) acid and/or salts	1327-53-3	0.1
9. Bromine	7726-95-6	20
10. Chlorine	7782-50-5	10

Etc. <https://www.legislation.gov.uk/uksi/2015/627/schedule/1/made>

Many of these exhibit dense-gas dispersion behaviour

# What causes density differences?

Molecular mass of gas relative to air





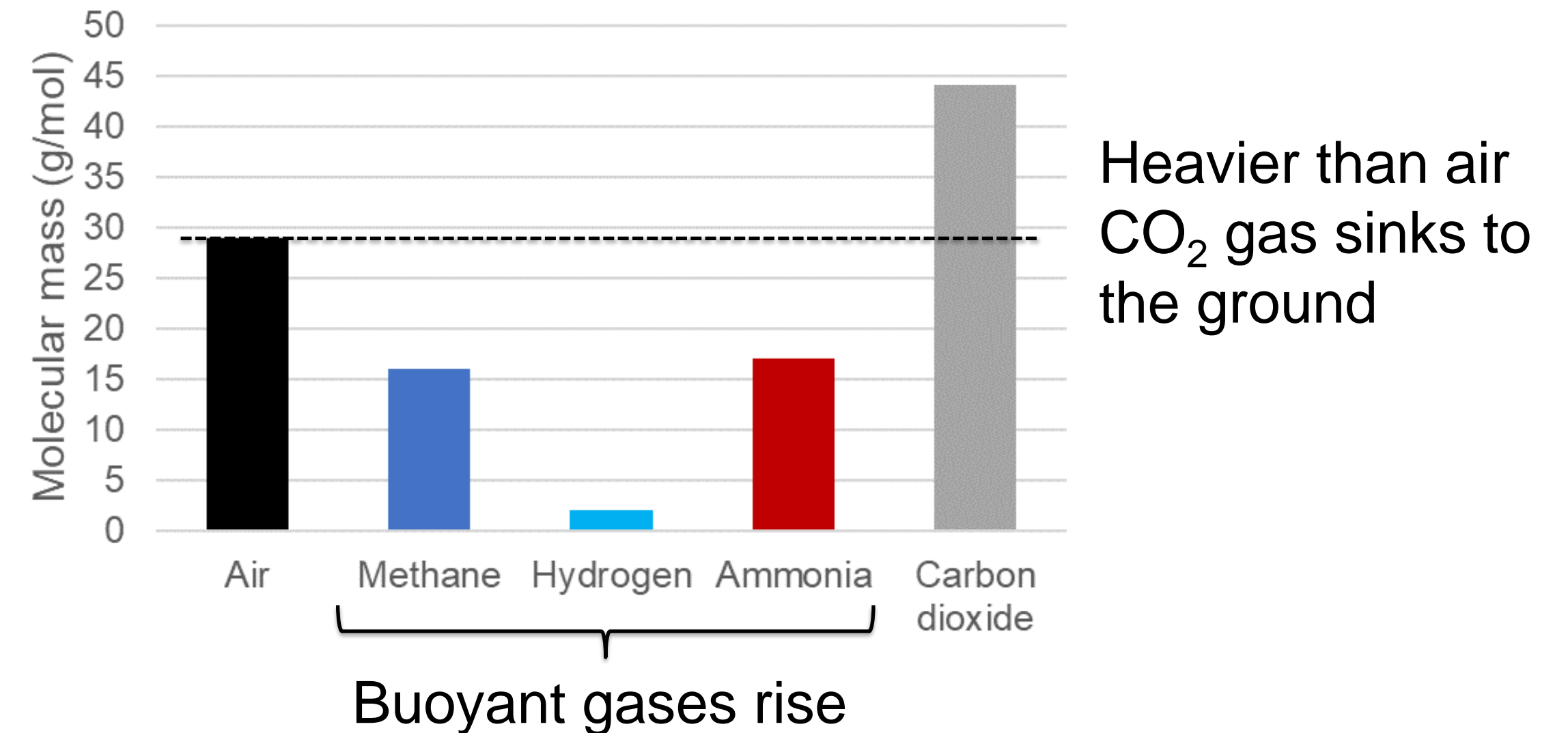
# What causes density differences?

Molecular mass of gas relative to air

**But...**

Temperature and aerosols are also important

Methane, hydrogen and ammonia can all behave as dense gases if they are cold and aerosols are present



Methane (liquefied natural gas)



<https://www.tradewindsnews.com/weekly/mol-outlines-lessons-learned-from-lng-ship-cargo-release/1-1-769623>

Hydrogen



Experiments at HSE for [www.preslhy.eu](http://www.preslhy.eu)

Ammonia



© DHS S&T CSAC [www.uvu.edu/es/jack-rabbit/](http://www.uvu.edu/es/jack-rabbit/)



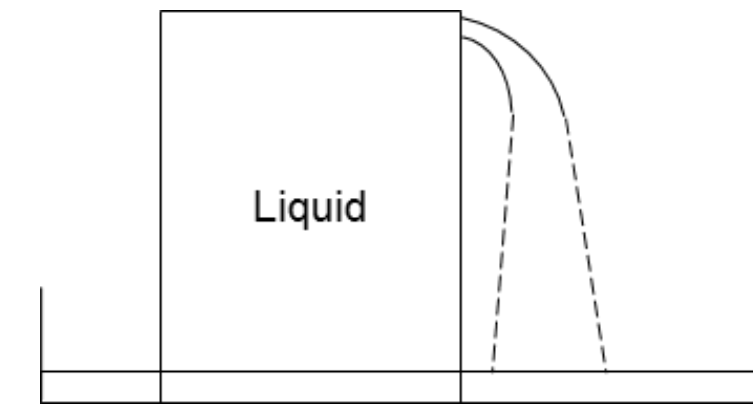
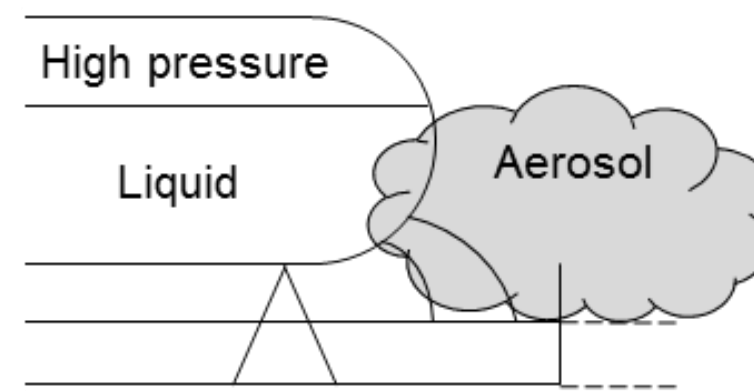
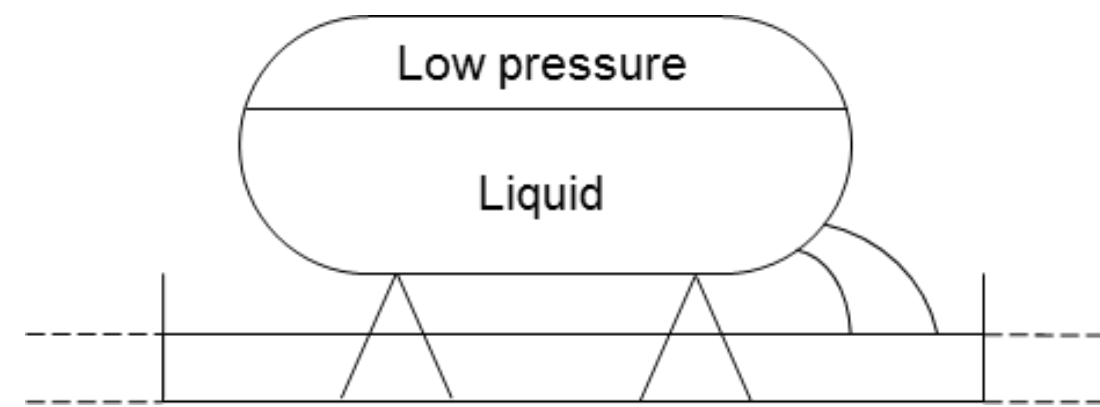
# Factors affecting dense gas dispersion

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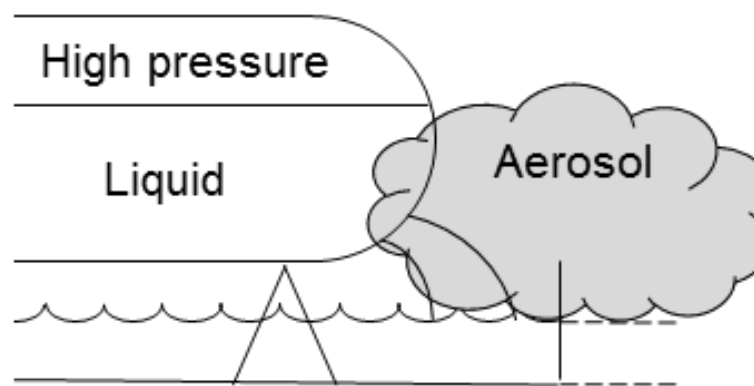
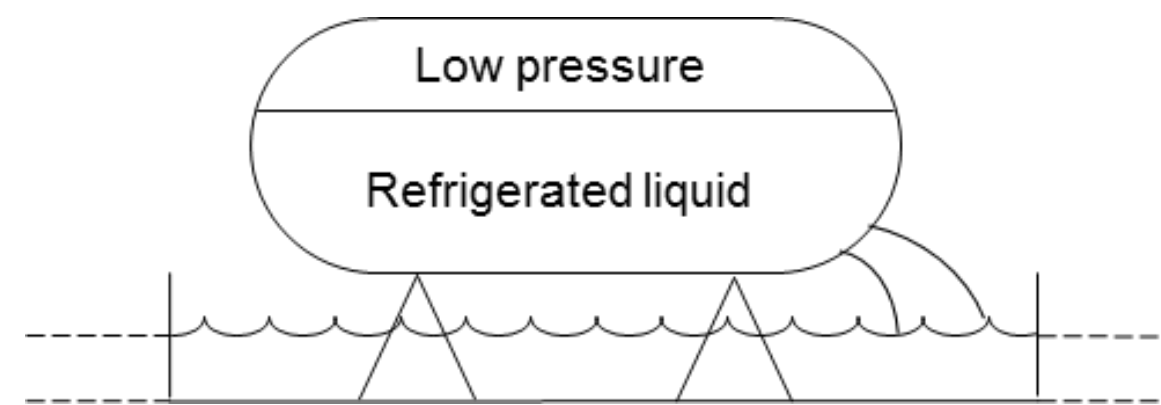
- Source geometry and conditions
- Atmospheric conditions (wind speed, stability, temperature)
- Heat transfer
- Phase changes
- Dry/wet deposition and surface chemical reactivity
- Surface conditions (roughness and obstacles)
- Topography

# Source conditions

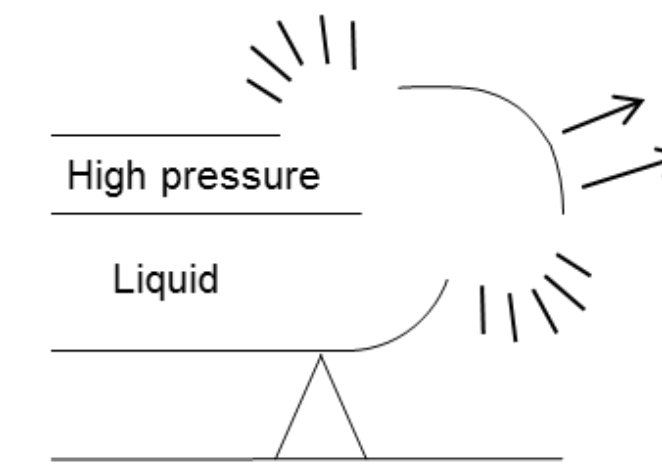
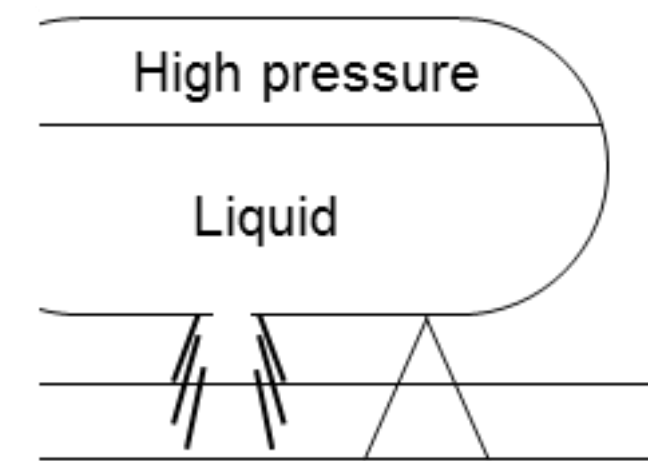
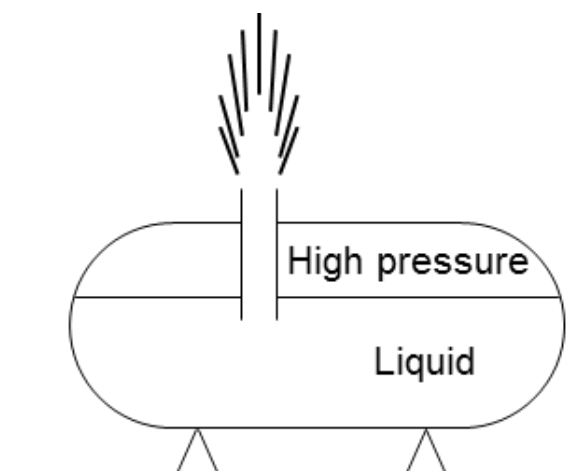
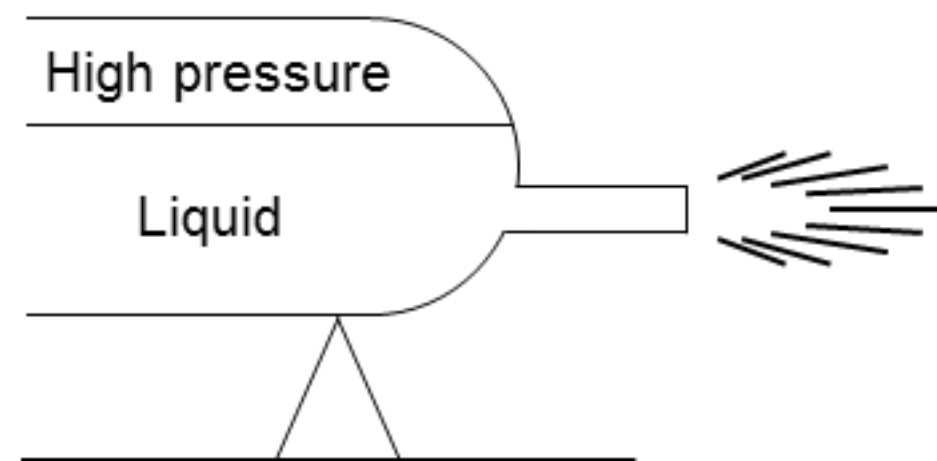
## Spills of liquids with boiling point above ambient temperature



## Spills of refrigerated liquids



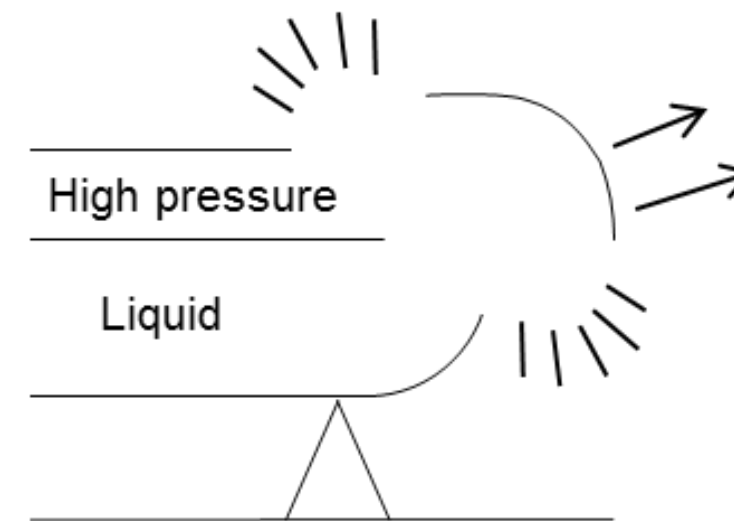
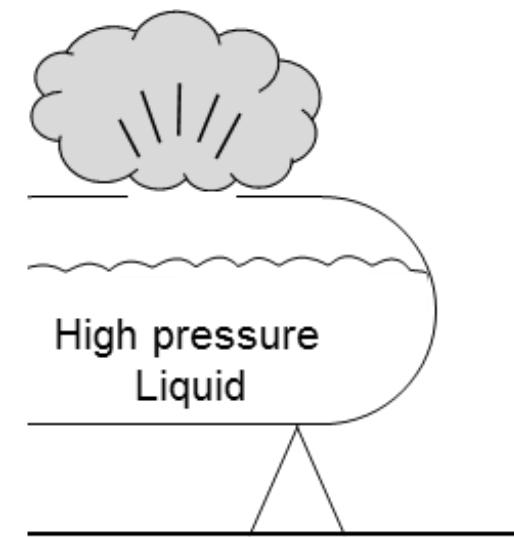
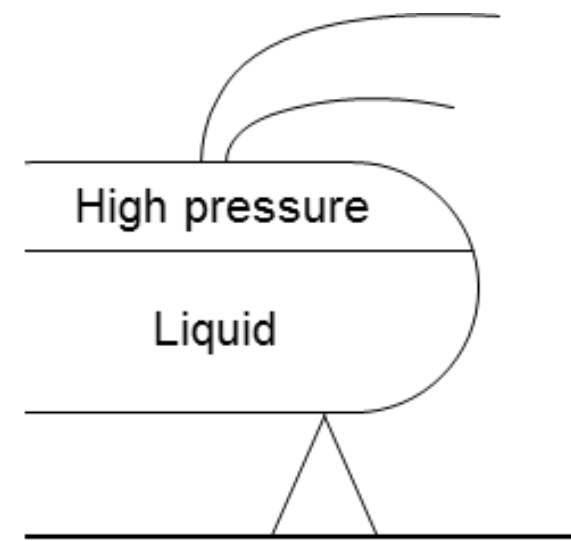
## Releases of pressure-liquefied gases



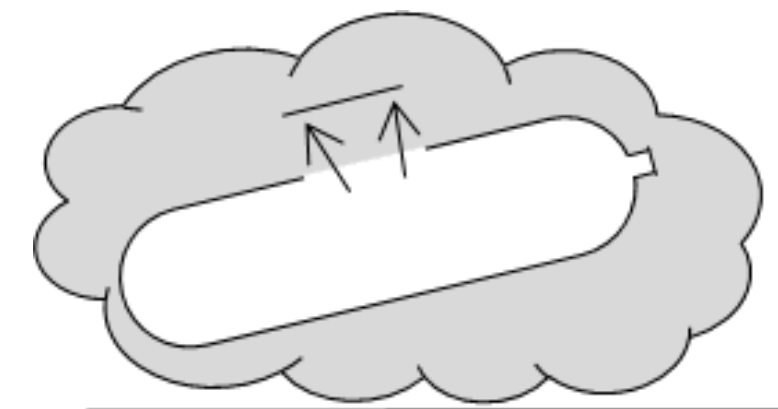
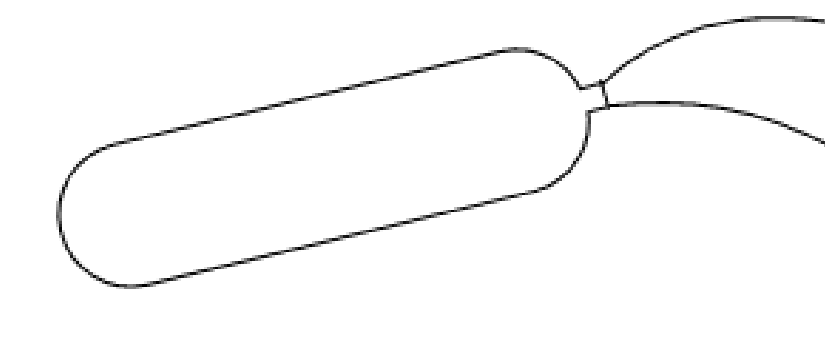
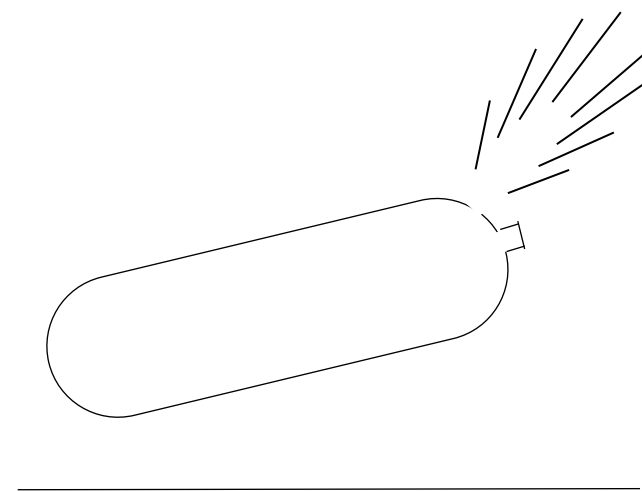
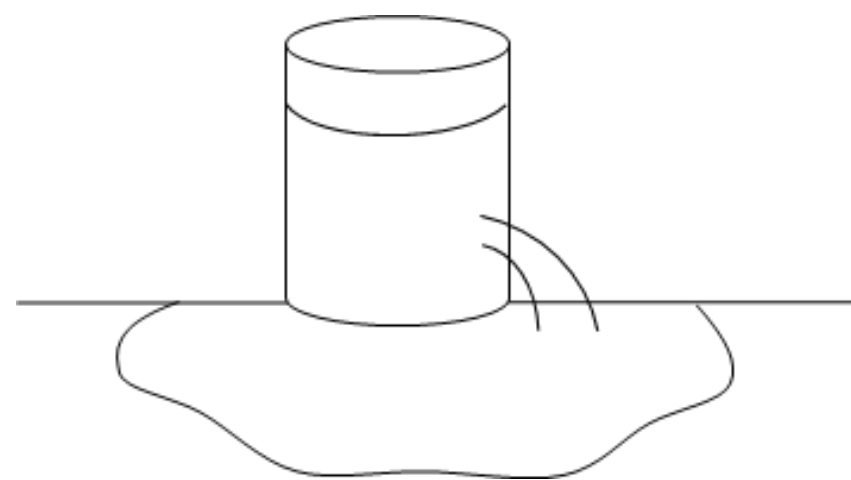
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## ... more source conditions

### Releases of pressurised vapour

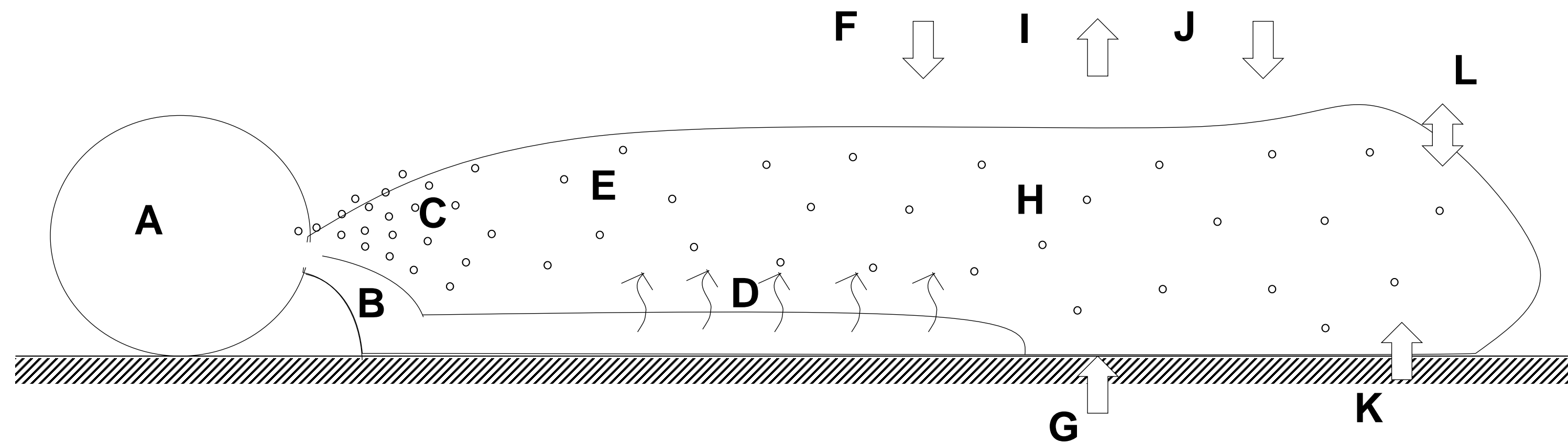


### Releases from drums and cylinders



Reactions of some chemicals can also produce dense gases, e.g.,  
acids + hypochlorites = chlorine gas

# Heat transfer and phase change



- |   |  |   |  |
|---|--|---|--|
| A | Ruptured vessel  | G | Ground heat flux to the surface                |
| B | Liquid spill   | H | Heat gain/loss due to condensation/evaporation |
| C | Cold temperature gas/aerosol mixture                                       | I | Heat loss due to radiation                     |
| D | Evaporation and possibly aerosols thrown into the cloud by violent boiling | J | Solar energy input                             |
| E | Endothermic or exothermic chemical reactions                               | K | Convective heat flux from surface to the plume |
| F | Entrainment of warm ambient air, subsequent condensation of water vapour   | L | Heat exchange by convection                    |

(Based on Hanna *et al.*, 1996)



# Characterisation of dense gas behaviour

- Froude number  $Fr = \frac{u}{\sqrt{g'L}}$  or in some references  $Fr = \frac{u^2}{g'L}$   $\frac{\text{Inertial forces}}{\text{Gravitational forces}}$
- Richardson number  $Ri = \frac{g'L}{u^2}$  where  $g' = g \frac{(\rho_g - \rho_a)}{\rho_a}$  is the reduced gravity

## 3.5 Criteria for Effectively Passive Behaviour

Under what conditions might a release be analysed using correlations from passive dispersion experiments that are widely available, have been well studied and exist in workbook form already (e.g. Turner, 1970; Clarke, 1979)?

For continuous releases of  $q_o m^3/s$  we recommend on the basis of Appendix A that the flow will be effectively passive and passive dispersion results may be used when

$$\left(\frac{g_o' q_o}{U_{ref}^3} / D\right)^{\frac{1}{3}} \leq 0.15$$

where  $U_{ref}$  is the velocity at  $z = 10$  m.

For an instantaneous release of  $Q_o m^3$  we recommend, also on the basis of Appendix A, that the flow will be effectively passive and passive dispersion results may be used when

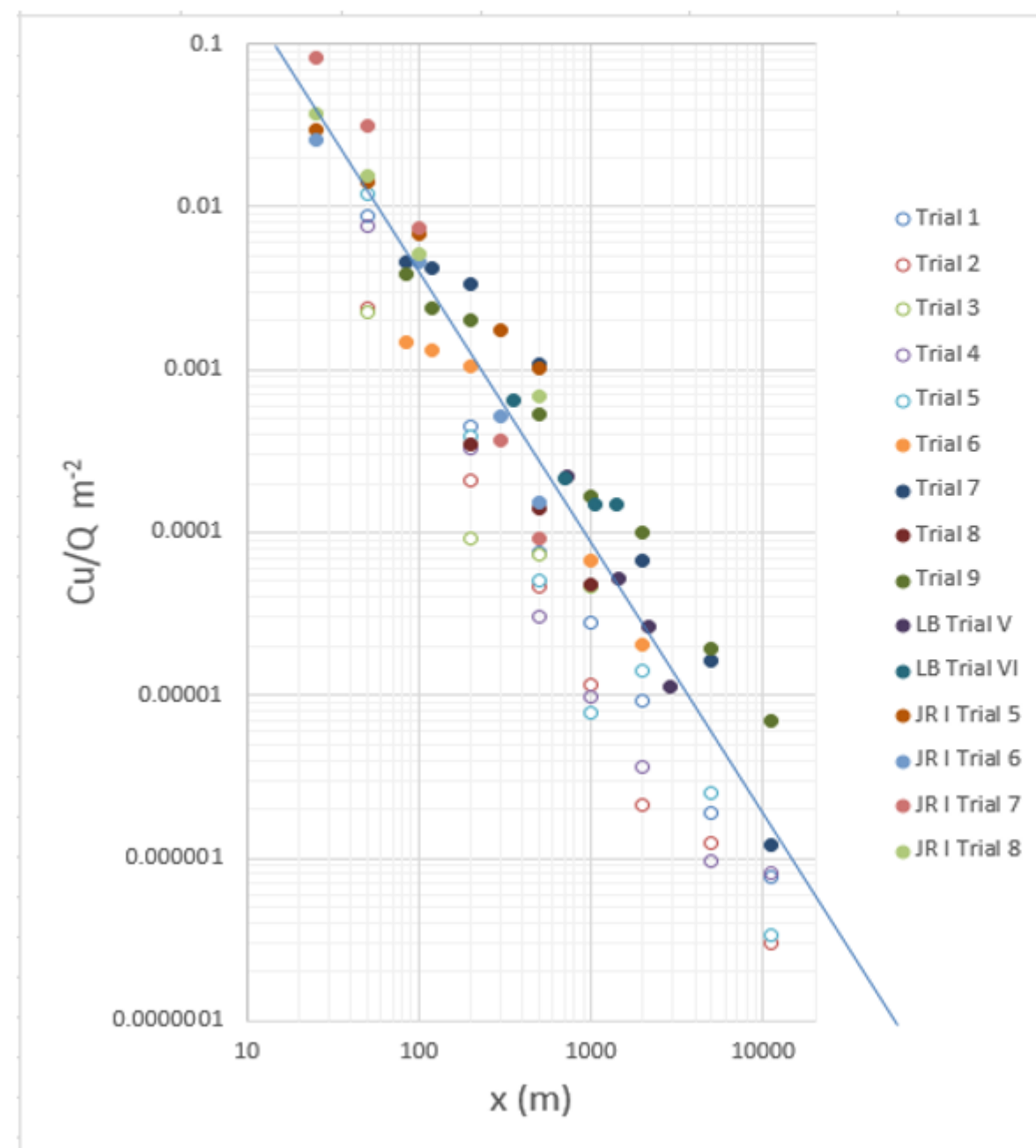
$$\frac{(g_o' Q_o^{\frac{1}{3}})^{\frac{1}{2}}}{U_{ref}} = \left(\frac{g_o' Q_o}{U_{ref}^2}\right)^{\frac{1}{2}} / Q_o^{\frac{1}{3}} \leq 0.2$$

where  $U_{ref}$  is again the velocity at  $z = 10$  m.

Source: Britter & McQuaid (1988) "Workbook on the dispersion of dense gases"  
<https://xnet.hsl.gov.uk/fileshare/public/3583/britter-mcquaid-1988-workbook-on-dense-gas-dispersion-crr88017.pdf>

# Decay of concentration with distance

## Arc max Cu/Q versus x for Lyme Bay (LB), Jack Rabbit I (JR I), and Jack Rabbit II (Trials 1 – 9)



The straight line represents the relation  $Cu/Q = 8.5x^{-5/3}$ , where  $Cu/Q$  has units  $m^{-2}$  and  $x$  has units  $m$

Source: Hanna, Chang & Mazzola (2017) “Analysis of Variations of Concentrations with Downwind Distance and Characteristics of Dense Gas Plume Rise for Jack Rabbit II–2015 and 2016 Chlorine Field Experiments”, Harmo-18

<https://www.harmo.org/conference.php?id=18>

## Theoretical basis supporting -5/3 power law decay of concentration by Jeff Weil

In previous work, Hanna et al. (2016b, 2017) found that the chlorine maximum surface concentrations from the 2015 Jack Rabbit II experiments decreased approximately as  $C_{max} \propto x^{-5/3}$ . This empirical correlation is presented later in the NCAR model comparisons with the Jack Rabbit II data and is derived below based on results from Appendix A.

The maximum concentration for an effective Gaussian distribution is proportional to the puff top-hat concentration  $C_{th}$  (Section 4.4), which is estimated from the puff radius  $R$  and depth  $h$  as  $C_{th} \propto Q/(R^2h)$ . At long times or far downstream,  $R \propto t^{3/5}$  and  $h \propto t$  and with  $C_{max} \propto C_{th}$ , the  $C_{max}$  is given by

$$C_{max} \propto Q/t^2 \quad (1)$$

A conversion from  $t$  to  $x$  as the independent variable can be made using the mean wind profile and the puff entrainment relationship at long times, where  $h \propto t$ . This  $h$  dependence means that the entrainment velocity  $w_e$  ( $= dh/dt$ ) must be constant.

We can also write

$$dh/dx = (dh/dt)/(dx/dt) = w_e / U(h) \quad (2)$$

where the mean wind is evaluated at  $z = h$ , and Eq. (2) can be rewritten as

$$U(h) dh = w_e dx \quad (3)$$

Now instead of using the logarithmic wind profile, we adopt a simple power-law profile of the form

$$U(z) = U_{ref} (z/z_{ref})^p \quad (4)$$

where  $U_{ref}$  is the reference wind speed at the reference height  $z_{ref}$ , and the exponent  $p$  is  $< 1$ .

By rewriting Eq. (4) as  $U(z) = a_1 z^p$  and substituting this along with  $z = h$  into Eq. (3), we can integrate the latter to obtain

$$h^{1+p} = [w_e (1 + p)]/a_1 \cdot x \quad (5a)$$

or

$$h = b_1 x^{-1/(1+p)} \quad (5b)$$

where  $b_1 = f(w_e, p, a_1)$ . Far downstream, we have  $h = w_e t$  and by using this in Eq. (5b), we find

$$t = (b_1/w_e) x^{-1/(1+p)} \quad (6)$$

The above relationship can be substituted into Eq. (1) to obtain

$$C_{max} \propto Q x^{-2/(1+p)} \quad (7)$$

For neutral conditions and a typical exponent  $p = 1/6$  (Counihan (1975); Irwin (1979), with  $z_0 = 0.1$  m), the exponent on  $x$  is  $-1.71$  and for  $p = 1/7$ , it is  $-1.75$ . These  $x$  exponents are close to the empirically-determined value of  $-5/3$ , and for a slightly more stable environment

<https://doi.org/10.1016/j.atmosenv.2018.08.009>



# Decay of concentration with distance

Complex behaviour in some dense-gas dispersion experiments with momentum-dominated flow (jetting) and transition from dense to passive dispersion

## Desert Tortoise ammonia experiments

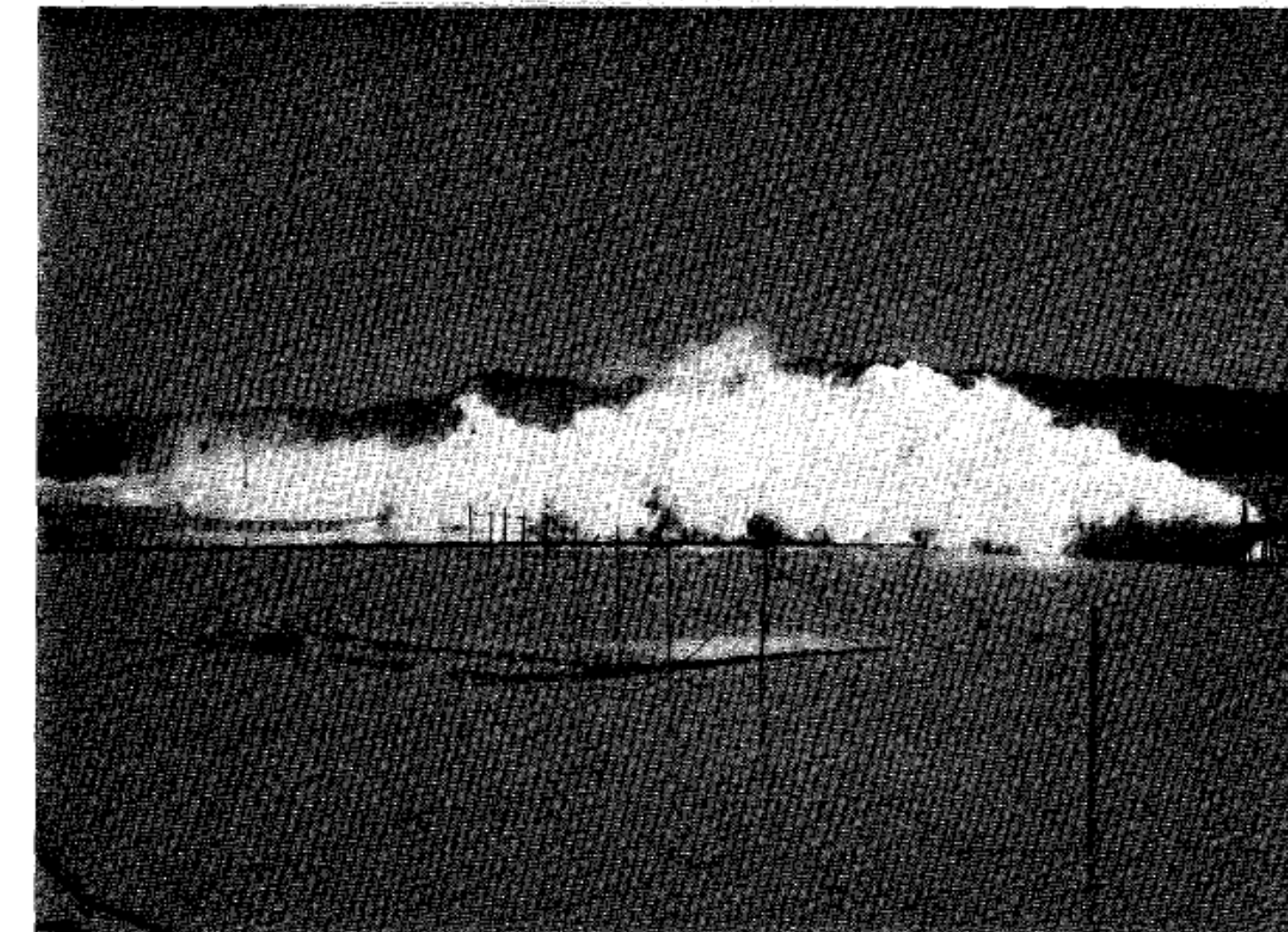
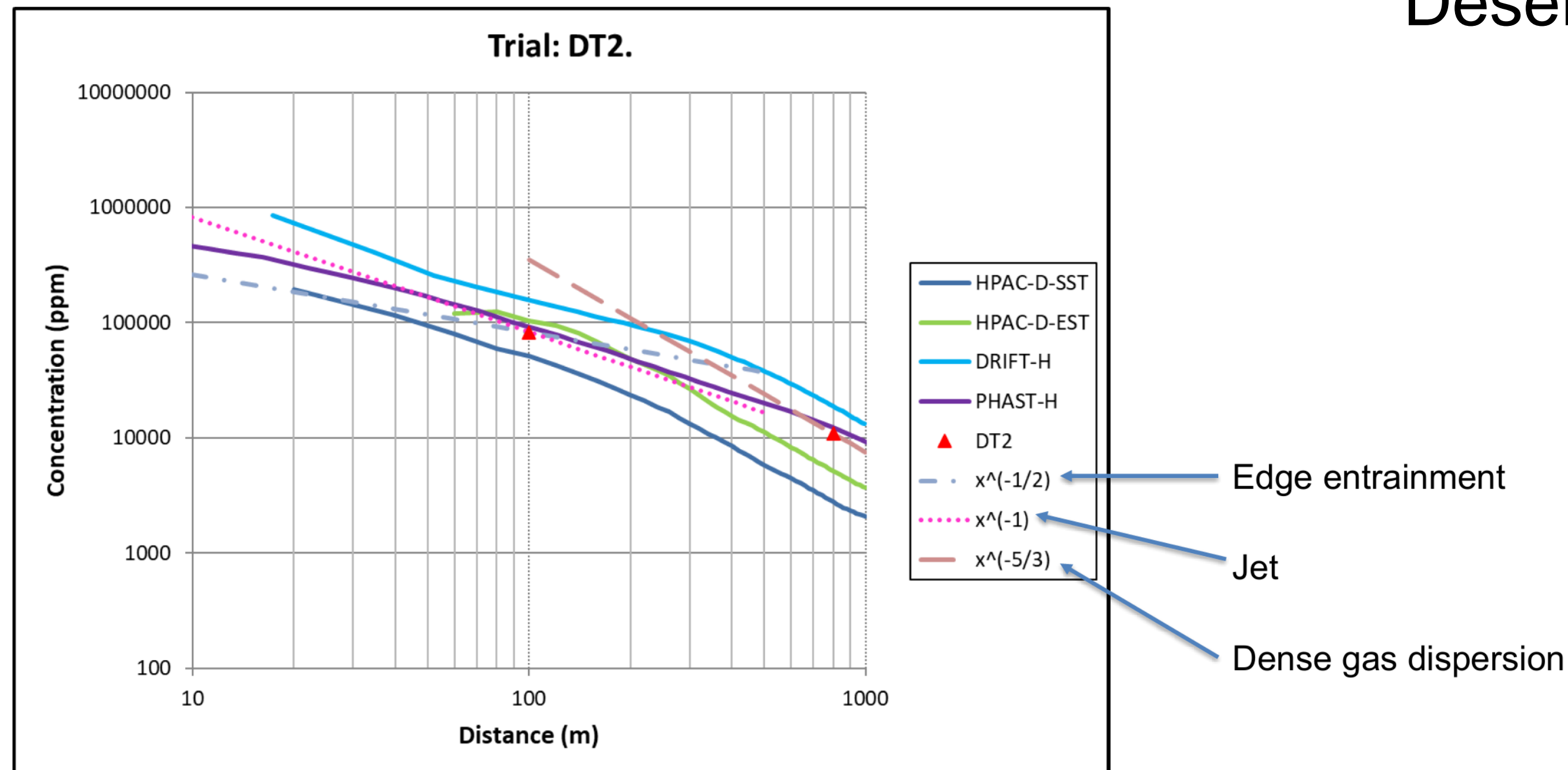


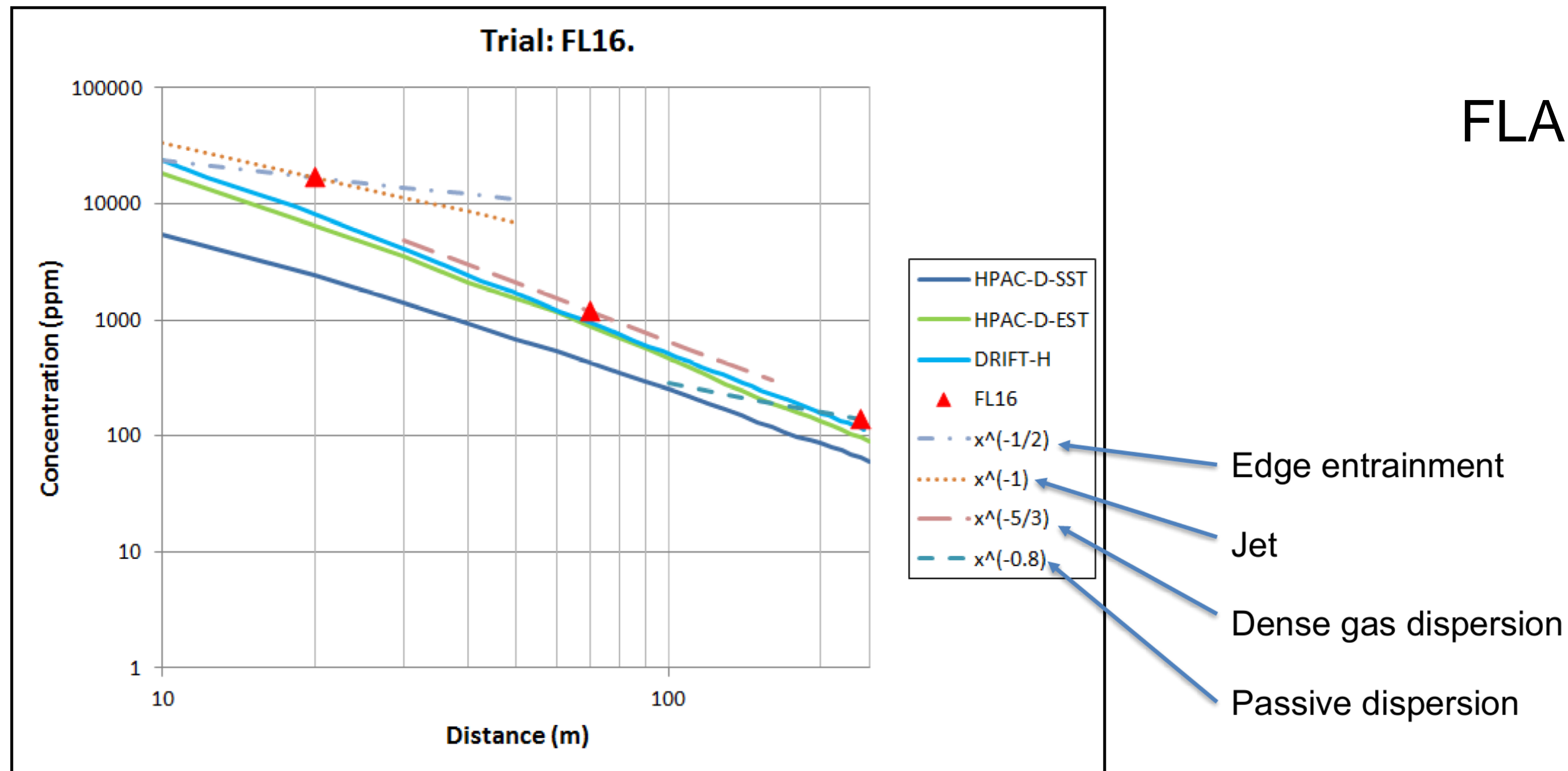
Fig. 15. Desert Tortoise 2 (upwind wide angle camera) Time = 230s. Lawrence Livermore National Laboratory

© LLNL <https://www.osti.gov/biblio/6393901>



# Decay of concentration with distance

Complex behaviour in some dense-gas dispersion experiments with momentum-dominated flow (jetting) and transition from dense to passive dispersion



## FLADIS ammonia experiments



Nielsen M. and S. Ott, 1996: FLADIS field experiments: final report, Risø-R-898(EN), Risø National Laboratory, Roskilde, Denmark, July 1996



# Decay of concentration with distance

For passive dispersion

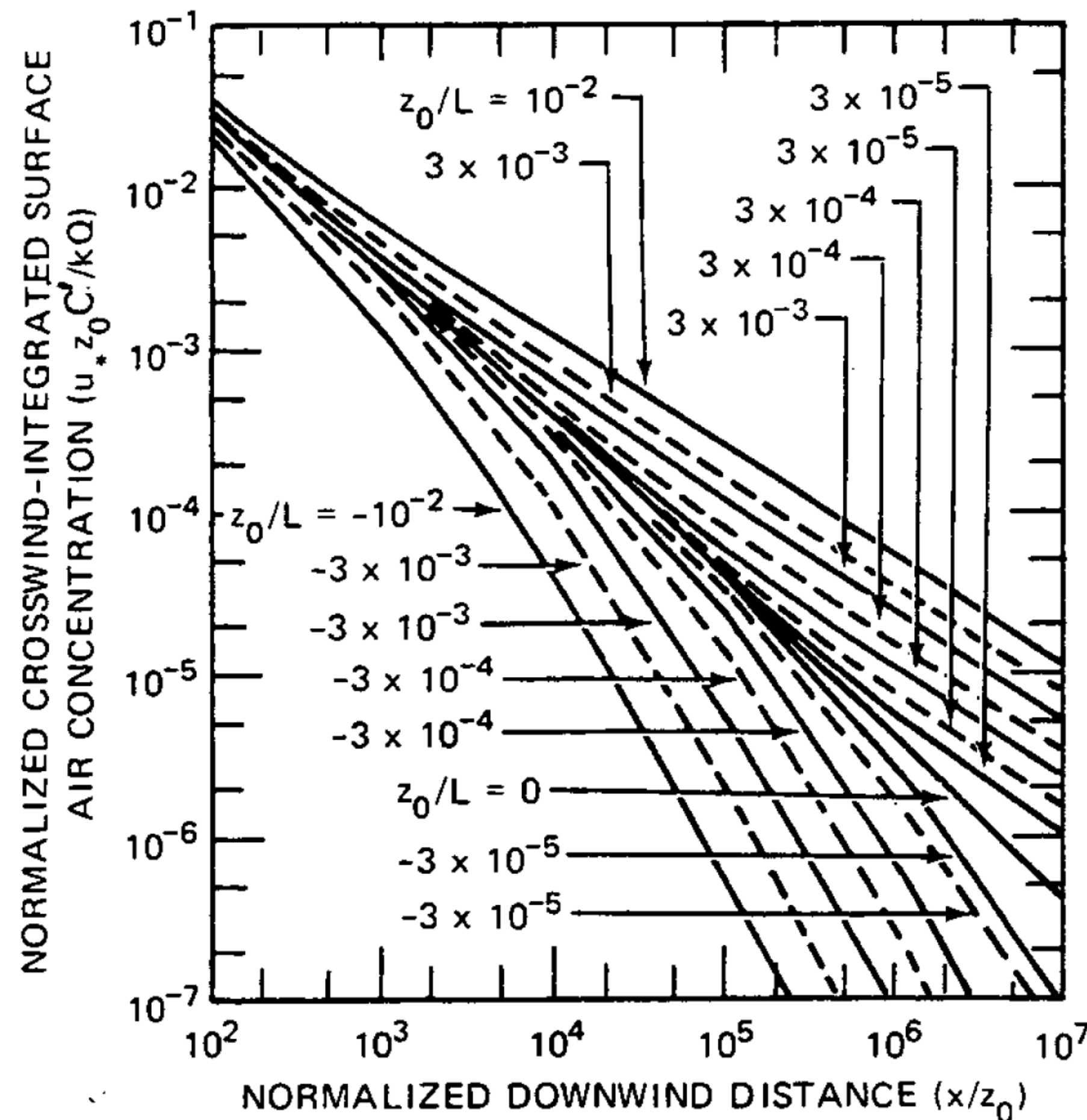


Fig. 7.2 Predicted crosswind-integrated concentration at ground level as a function of downwind distance for various stability conditions. [From T. W. Horst, Lagrangian Similarity Modeling of Vertical Diffusion from a Ground Level Source, *J. Appl. Meteorol.*, 18: 734 (1979).]

Source: Hanna, Briggs & Hosker "Handbook of atmospheric diffusion" <https://www.nrc.gov/docs/ML0926/ML092640175.pdf>

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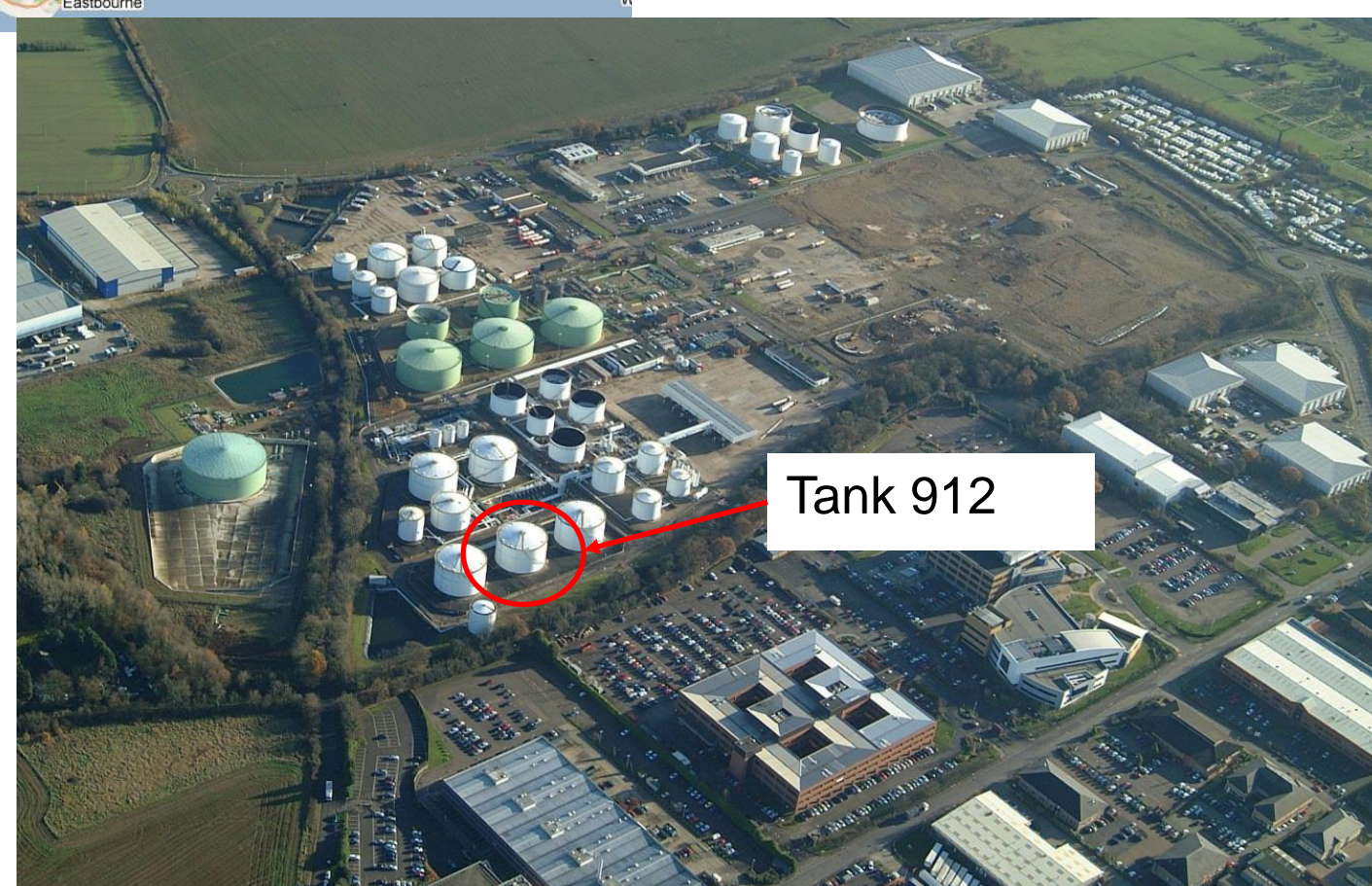
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- Ongoing HSE research activities



# Buncefield, UK (2005): Gasoline vapour

- Incident caused by overfilling a gasoline bulk storage tank





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Tower 8



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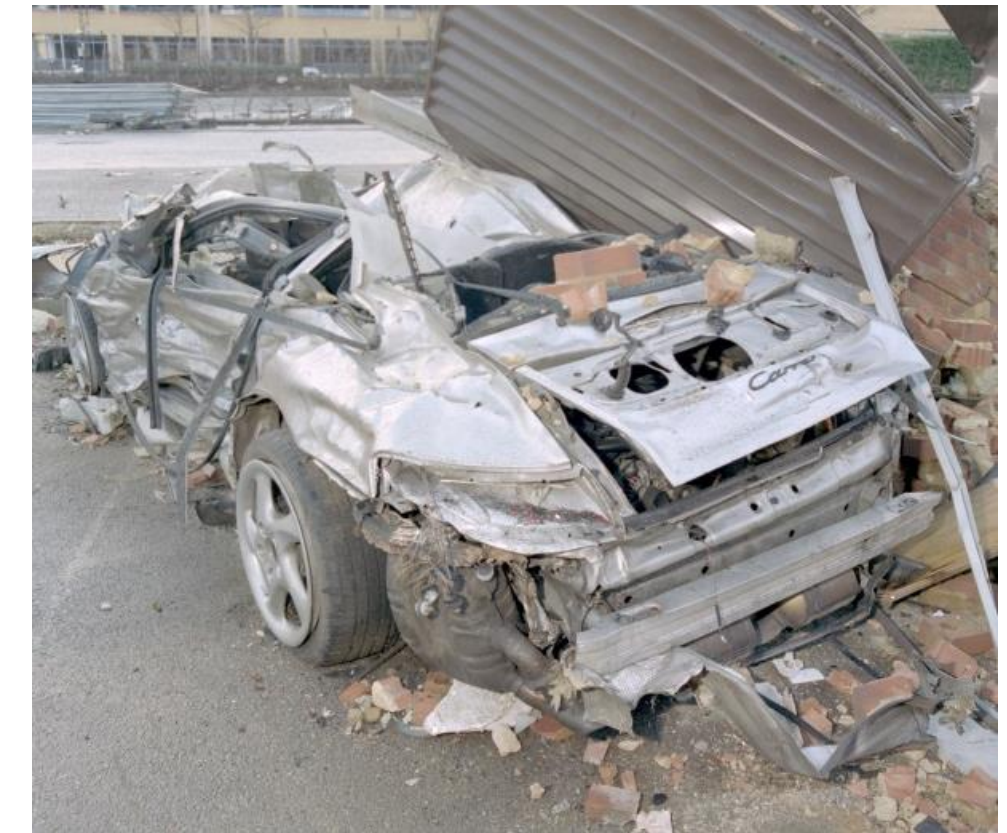
Tower 8







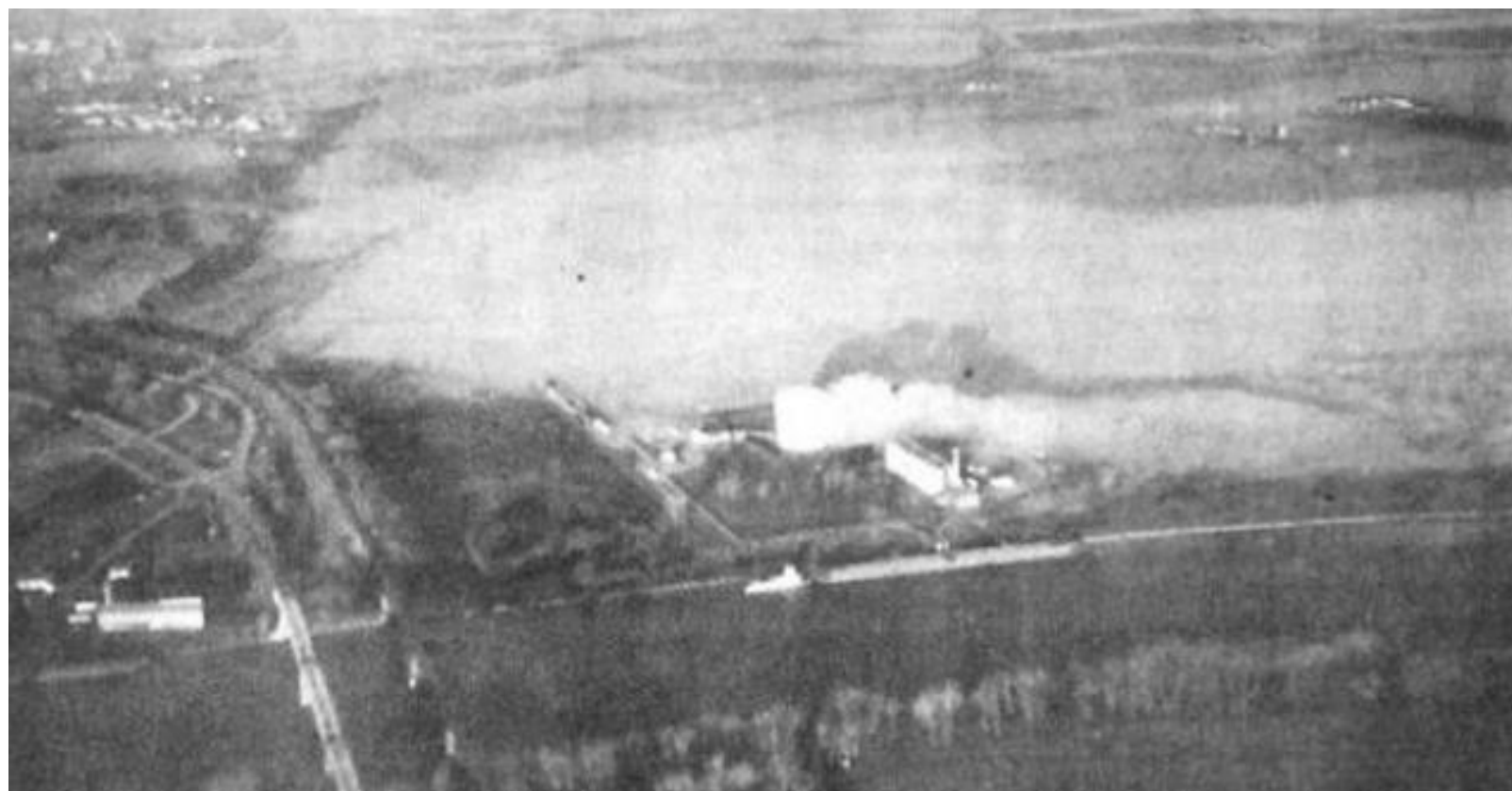
# Buncefield, UK (2005): Gasoline vapour





# Blair, Nebraska (1970): Ammonia

- Overflow of ammonia from 36,000 t refrigerated storage tank
- Tank levels not carefully monitored, alarm and shut-down system failed to operate
- Overflow discharge valve failed to operate at the set pressure, so that the liquid level in the tank rose until it reached the roof, at which point the overflow valve did open
- Discharge continued for 2.5 h, producing a dense vapour cloud that blanketed the surrounding area, 10 m thick and extending to a distance of 2.7 km
- Cloud eventually dispersed and avoided populated areas, three people hospitalised



The Enterprise newspaper, 1 October 2004, [www.blairnebraska.com](http://www.blairnebraska.com)



Photos kindly provided by Steven Hanna (originally from Rex Britter)  
See also: Lees Loss Prevention, ISBN: 978-0-12-397189-0



# Houston, Texas (1976): Ammonia

- Road tanker crashed through highway bridge rail at intersection
- Vessel holding 19 t of pressure-liquefied ammonia ruptured on impact
- Dense cloud of ammonia vapour covered an area of 300 m x 600 m
- 100 people injured, 6 deaths



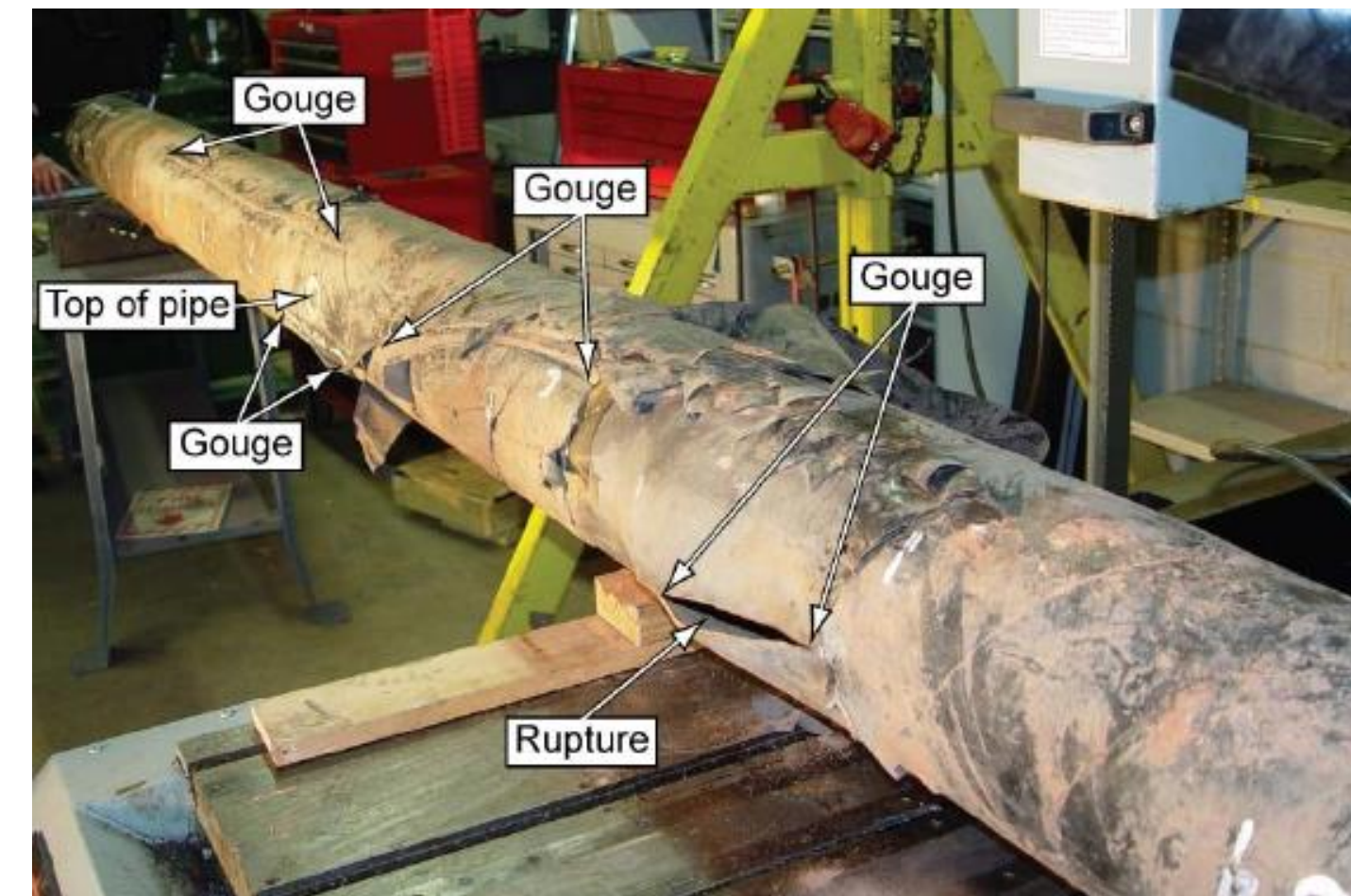
<https://www.houstonchronicle.com/news/houston-texas/houston/article/In-1976-an-ammonia-truck-disaster-claimed-the-12906732.php>

Photograph taken by Texas Air Control Board  
© Texas Commission Environmental Quality copyright 1976



# Kingman, Kansas (2004): Ammonia

- 8-inch diameter Magellan pipeline ruptured and released 480 t of ammonia
- Visible vapour cloud 0.5 miles wide and 1.5 miles long
- Four families evacuated, no injuries
- Analysis showed pipeline rupture was caused by damage from digging equipment, either during construction or later agricultural activities



<https://www.nts.gov/investigations/AccidentReports/Reports/PAB0702.pdf>



# Beach Park, Illinois (2019): Ammonia

- Release of 1.5 t of ammonia from faulty coupling on two 1,000-gallon nurse tanks being towed by a tractor in farming area
- Vapour dispersed in dense cloud: 1 mile shelter-in-place order imposed
- 83 people taken to hospital, 14 admitted, 8 in intensive care unit, no deaths



<https://www.nts.gov/investigations/AccidentReports/Reports/HZIR2201.pdf>

<https://www.cbsnews.com/chicago/news/ammonia-spill-beach-park/>

<https://www.chicagotribune.com/suburbs/lake-county-news-sun/ct-Ins-ammonia-spill-no-charges-st-0626-20190625-ikztowshfhwhgym3lryjk4v2m-story.html>



## Festus, Missouri (2002): Chlorine

- 20 t of chlorine released due to failure of a transfer hose from railcar
- 63 people sought medical attention, 3 hospitalised, no fatalities



KTVI-TV, St. Louis, Missouri



KTVI-TV, St. Louis, Missouri

<https://www.csb.gov/dpc-enterprises-festus-chlorine-release/>



# Jordan Aqaba Port (2022): Chlorine

- Catastrophic failure of chlorine storage tank dropped during a lifting operation



Video broadcast by state-owned AlMamlaka TV showed the dock engulfed in a cloud of yellow gas



<https://www.bbc.co.uk/news/world-middle-east-61950965>

<https://www.youtube.com/watch?v=DfR1K9c6lUA>



# Chelyabinsk, Russia (2011): Bromine

- 24-50 litres of bromine released from glass containers damaged during movement of railway carriages
- 47 people received medical treatment



<https://www.youtube.com/watch?v=OszlK-1xxuA>

<https://www.bbc.co.uk/news/world-europe-14755874>

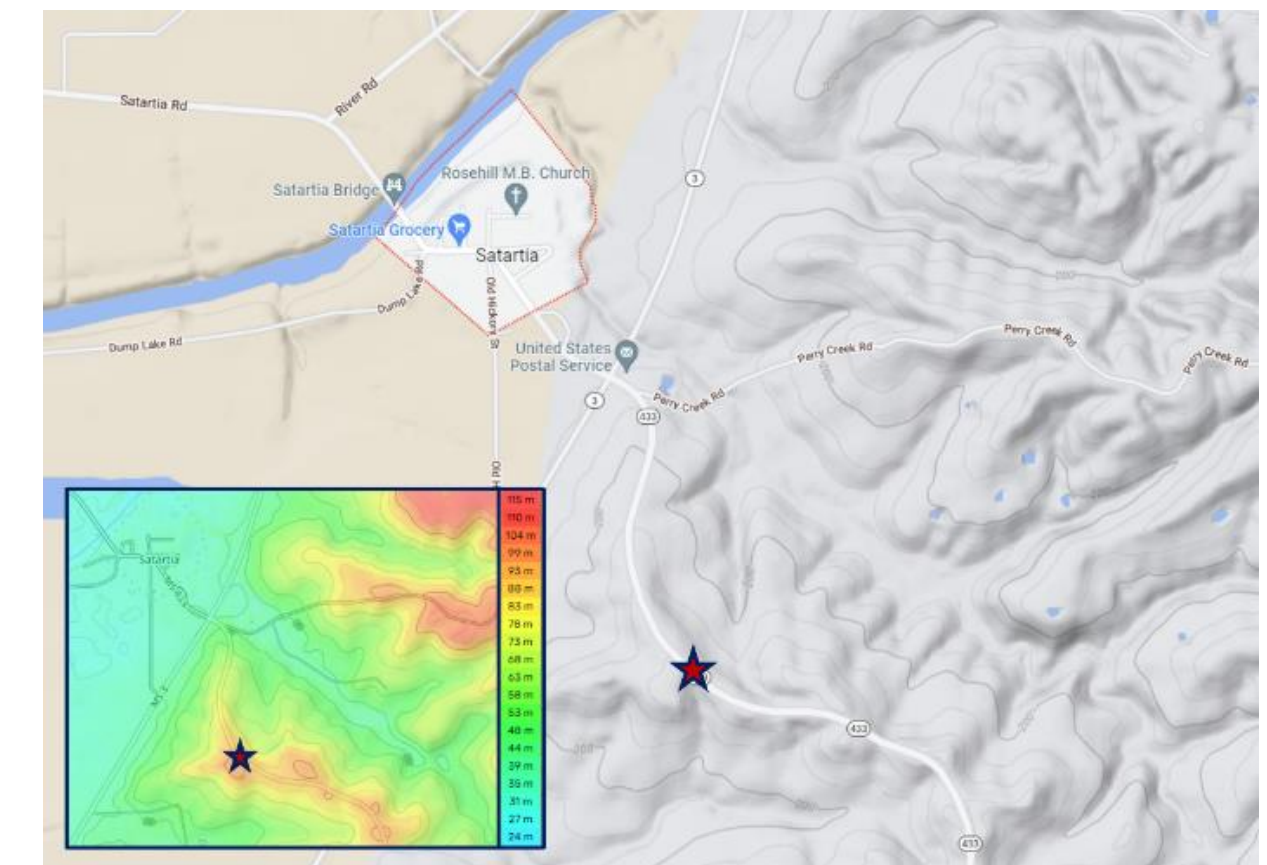


# Satartia, Mississippi (2020): Carbon dioxide

- Failure of Denbury 24-inch CO<sub>2</sub> pipeline near Satartia, Mississippi due to landslide
- Dense CO<sub>2</sub> cloud rolled downhill and engulfed Satartia village, a mile away
- Approximately 200 people evacuated and 45 required hospital treatment
- Communication issues: local emergency responders were not informed by pipeline operator of the rupture and release of CO<sub>2</sub>
- Denbury's risk assessment did not identify that a release could affect the nearby village of Satartia



Figure 6: Topographical Map Showing the Delhi Pipeline (Green) and Denbury's Buffer Zone (Red) on Either Side of the Pipeline and the Proximity to Satartia (Blue Star Indicates the Rupture Site)



Terrain map taken from Google Maps and contour map taken from topographic-map.com. Approximate location of release marked by a star.



# Lake Nyos, Cameroon (1986): Carbon dioxide

- Release of 100kt -300kt of carbon dioxide from lake within volcanic crater
- Dense cloud rolled down valley and killed 1,746 people

<https://www.atlasobscura.com/places/lake-nyos-the-deadliest-lake-in-the-world>



<https://www.voanews.com/a/survivors-1986-lake-nyos-disaster-cameroon/3474673.html>

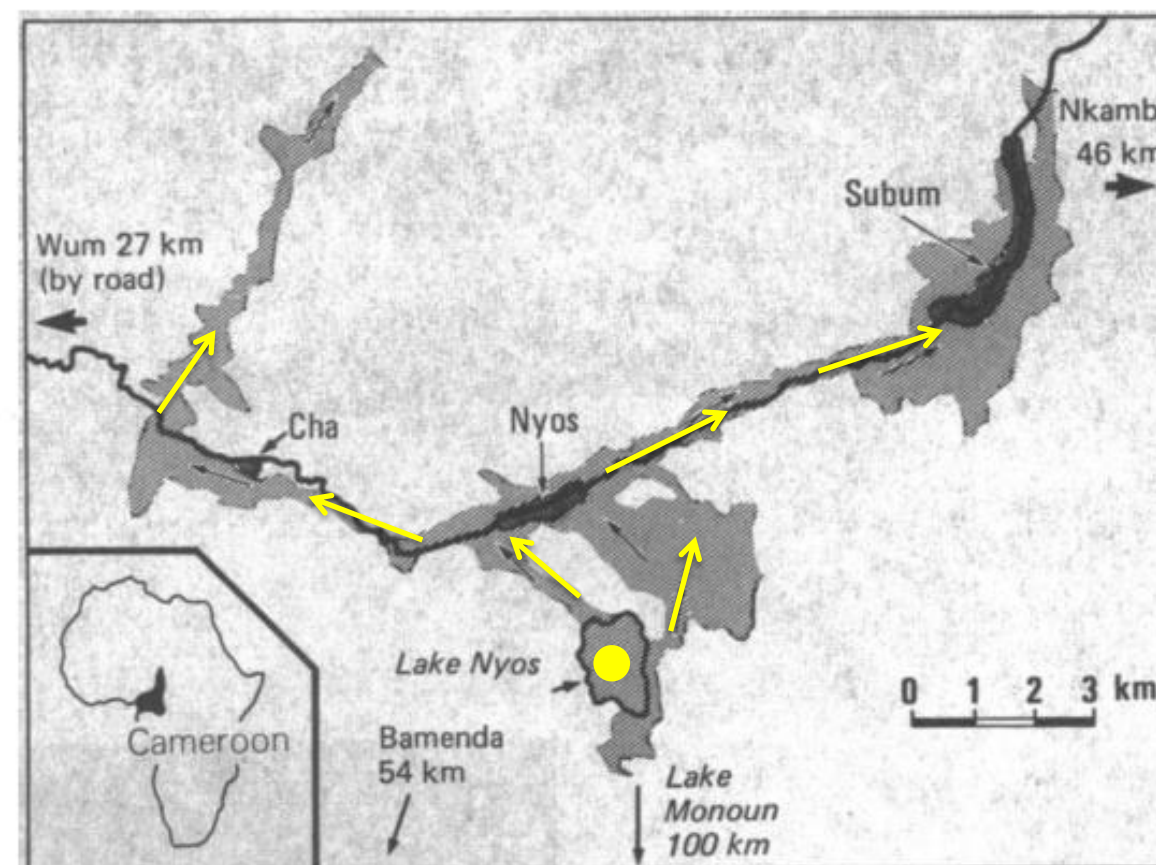


FIG 1—Direction of flow of gas (arrows; stippled area) from Lake Nyos into adjacent valleys

Baxter et al. (1989), © BMJ Publishing Group Ltd.

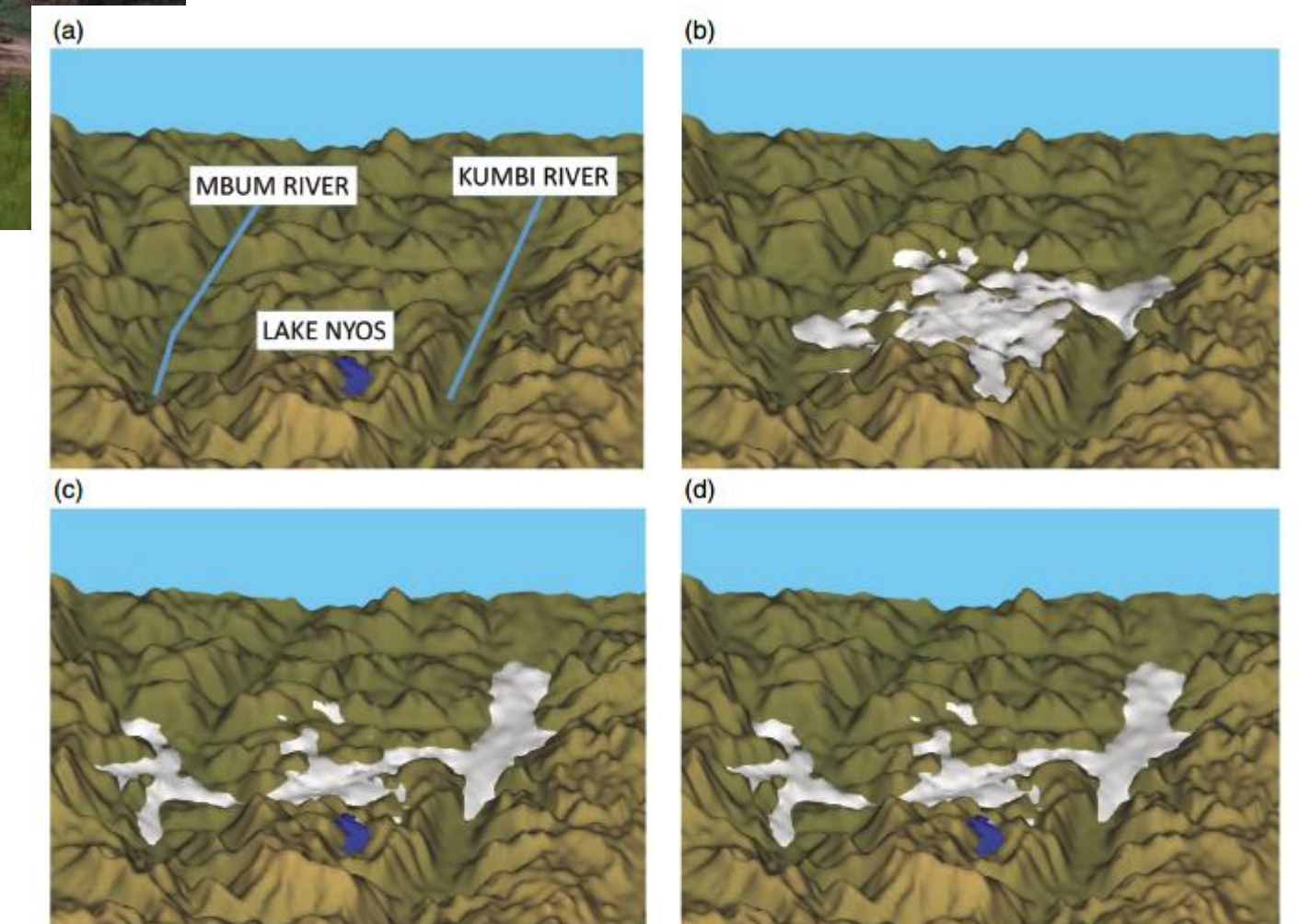


Figure 8. Three-dimensional visualization of the simulated spread of CO<sub>2</sub> from Lake Nyos. (a) Before eruption and (b) 20, (c) 40 and (d) 60 min after eruption. The 5% CO<sub>2</sub> concentrations in all plots represent the threshold level where the onset of laboured breathing occurs. The plots are designed to simulate a viewpoint from an elevated position, looking due north.

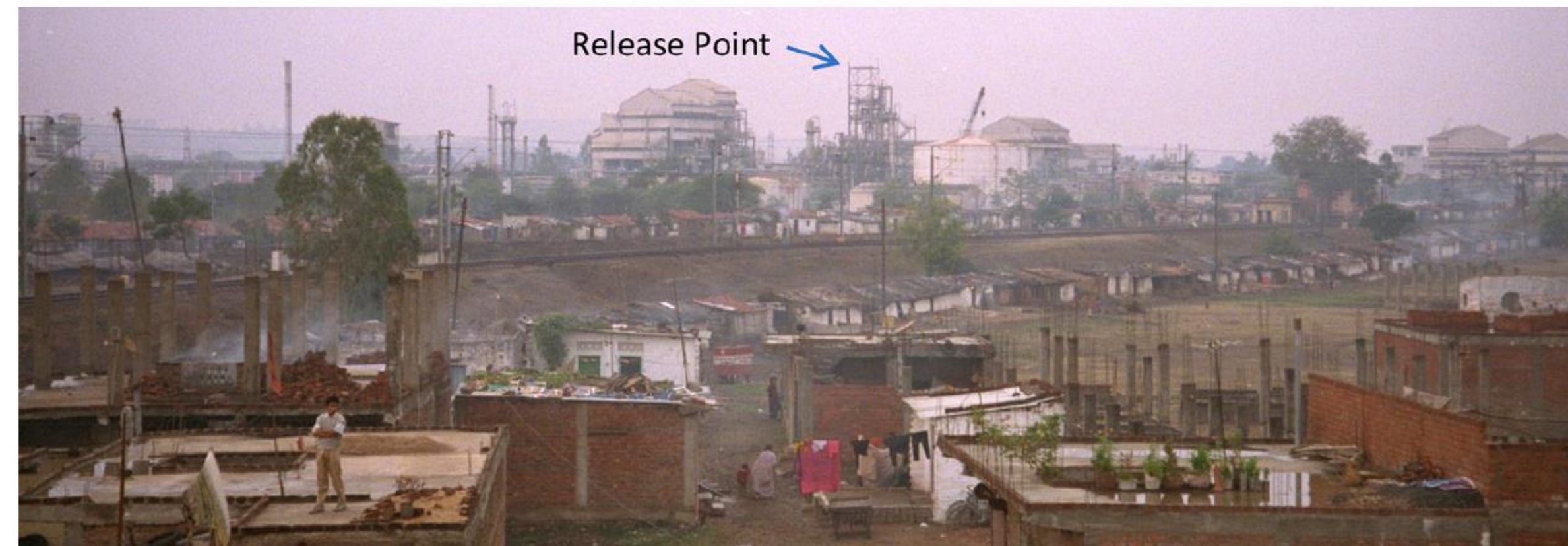
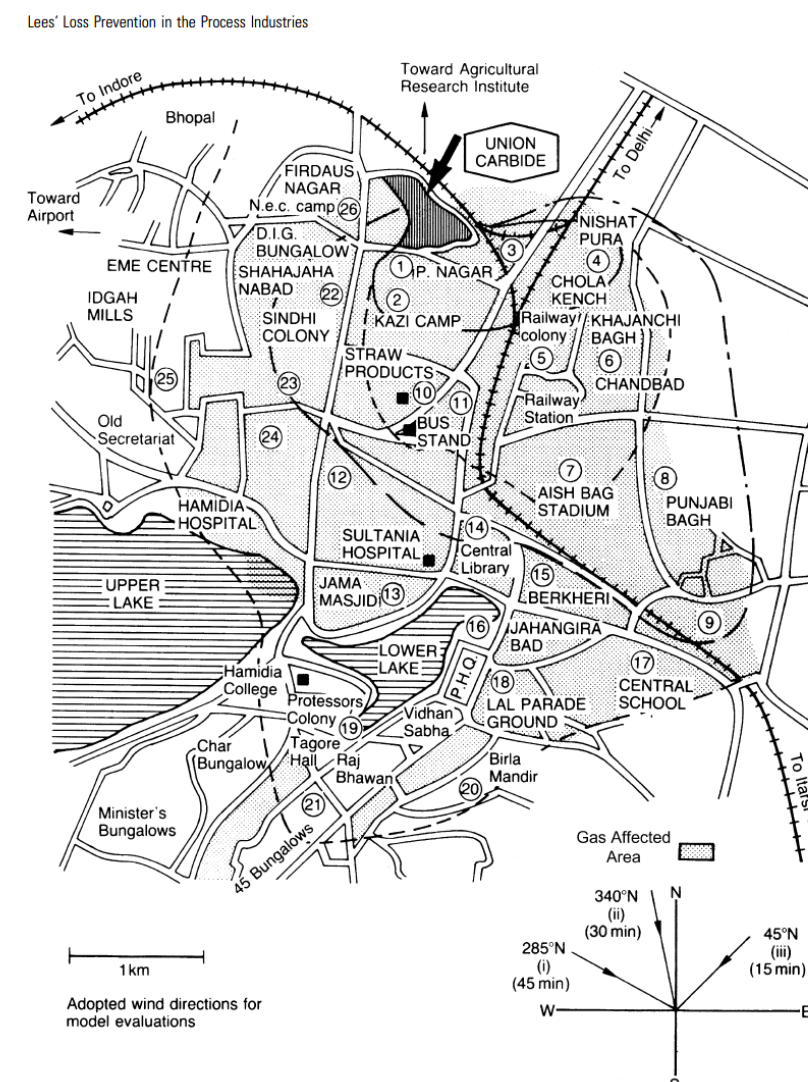
<http://dx.doi.org/10.1002/met.1603>



# Bhopal, India (1986): MIC

- Pressure relief valve released highly toxic methyl isocyanate (MIC) from chemical plant
- Cloud of MIC gas dispersed into housing and shantytowns close to the site
- Release occurred at night: light wind, stable inversion, toxic cloud hung around the area for the entire next day (AEGL-3 is just 0.4 ppm for 30 mins exposure)\*
- To date: 25,000 people died, 150,000 people with chronic illnesses
- Initial gas density ranges from 2.4 to 4.3 kg/m<sup>3</sup> in different assessments

<https://www.bhopal.net/>



Photograph by Jerry Havens – International Medical Commission to Bhopal, 1994.

<http://dx.doi.org/10.1016/j.jhazmat.2012.06.055>

<http://dx.doi.org/10.1016/j.atmosenv.2015.06.038>

\* <https://www.ncbi.nlm.nih.gov/books/NBK201335/>



# Review of dense gas incidents by Rachel Batt (2021)

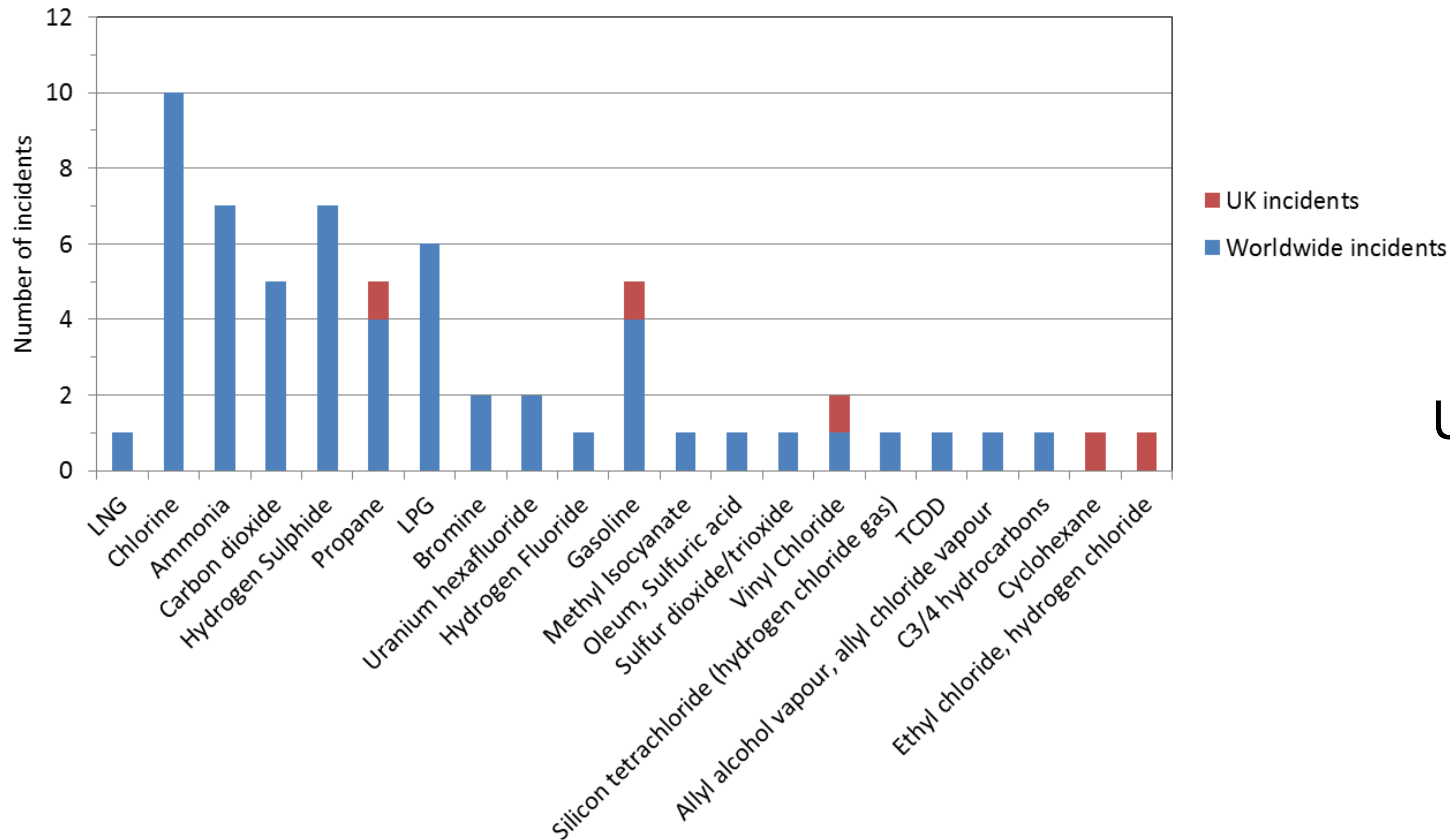
Name  
 Substance  
 Flammable  
 Toxic/health  
 Industrial  
 Off-site  
 Rural  
 Railcar  
 Road tanker  
 Pipeline  
 Ship  
 Off-shore  
 Indoor  
 Death  
 Injuries  
 Instantaneous  
 Continuous  
 Pressurised  
 Elevated

Liquid pool  
 Storage tank  
 overfilling  
 Catastrophic failure  
 Vent/valve  
 Pipe/hose  
 Puncture/crack/hole  
 Obstructions  
 Topography  
 Nil/low wind  
 Concentration data  
 Ingress  
 Mitigation  
 ER/safety reg  
 ignored/failed  
 Previous model  
 validation  
 Potential model  
 validation  
 Source description

Excel spreadsheet available here: <https://admlc.com/publications/>



# Substances involved in dense gas incidents



Top five substances worldwide:

- Chlorine
- Ammonia
- Hydrogen sulphide
- LPG
- CO<sub>2</sub>, propane & gasoline

UK incidents

- Propane
- Gasoline
- Vinyl chloride
- Cyclohexane
- Ethyl chloride / hydrogen chloride



# Other examples of gravity currents in nature



<https://wallpapercave.com/avalanche-nature-wallpapers>



<https://education.nationalgeographic.org/resource/pyroclastic-flow/>



<https://mymodernmet.com/arizona-dust-storm-news-helicopter/>

Also:

- Sea-breeze fronts
- Storm gust fronts
- Atmospheric bores
- Katabatic flows



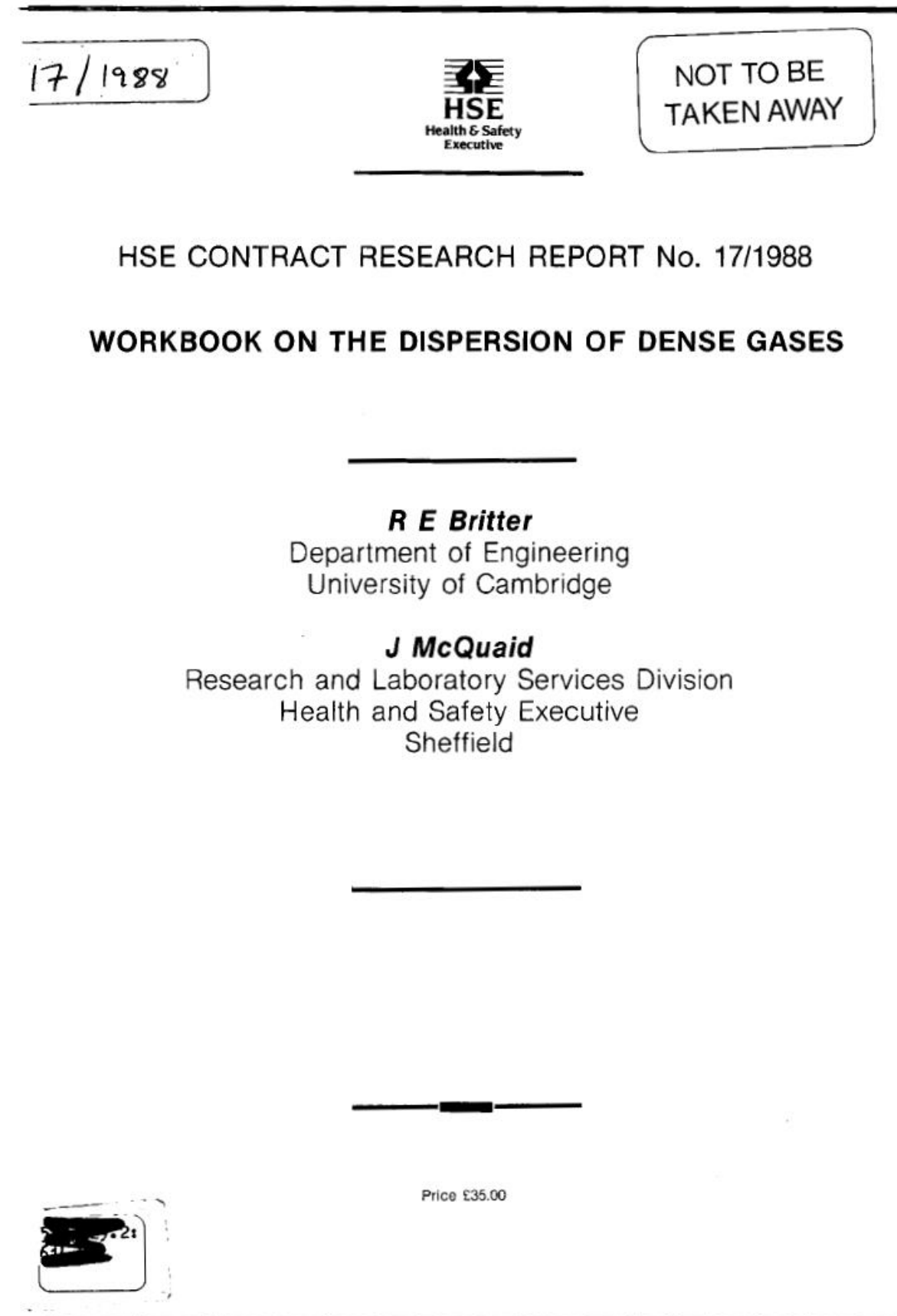
# Modelling approaches

---

- Empirical correlations and nomograms
- Integral
- Gaussian puff
- Lagrangian
- Computational Fluid Dynamics (CFD)
- Shallow layer
- Lattice-Boltzmann
- Smooth particle hydrodynamics



# Empirical nomograms



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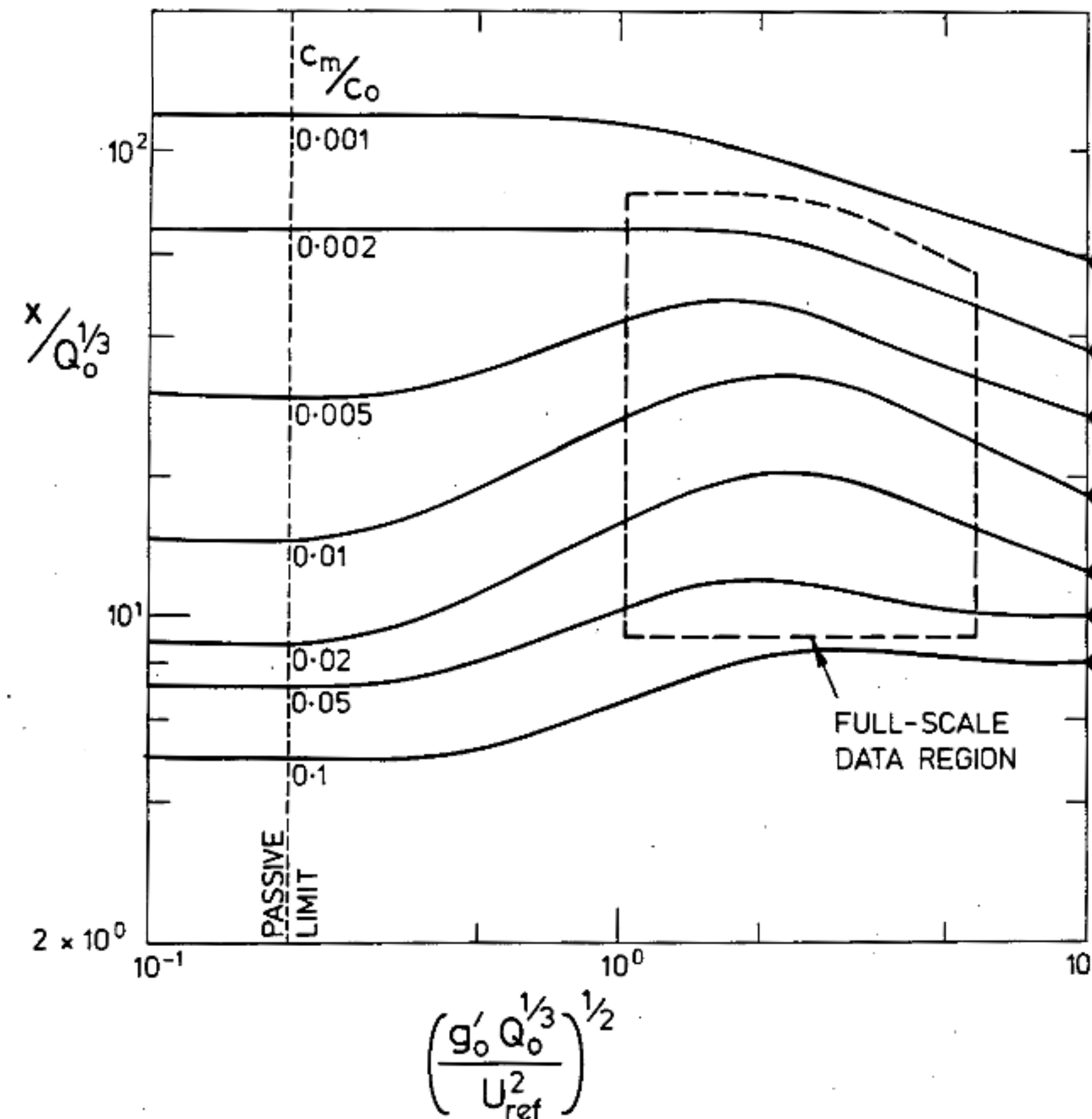
<https://xnet.hsl.gov.uk/fileshare/public/3583/britter-mcquaid-1988-workbook-on-dense-gas-dispersion-crr88017.pdf>



# Britter & McQuaid (1988) workbook

- Downwind distance to a particular concentration, for instantaneous releases

$Q_o$  source volume ( $m^3$ )  
 $x$  downwind distance (m)  
 $g_o$  reduced gravity at source ( $m/s^2$ )  
 $U_{ref}$  reference wind speed (m/s)  
 $C_o$  source concentration  
 $C_m$  ground-level concentration on plume axis





# German VDI 3783 Part 2 guidelines

<small>DK/UDC 602.55(203): 551.510.4: 551.511: 523.31-652-125 502.572: 620.28: 614.878: 628.395 351.777.078.33 614.711/75(083,132)</small>		
<b>VDI-RICHTLINIEN</b>		
<b>VEREIN DEUTSCHER INGENIEURE</b>	Umweltmeteorologie Ausbreitung von störfallbedingten Freisetzungen schwerer Gase – Sicherheitsanalyse  Environmental Meteorology Dispersion of Heavy Gas Emissions by Accidental Releases – Safety Study	<b>VDI 3783</b>  Blatt 2 / Part 2  Ausg. deutsch/englisch Issue German/English
<small>Juli 1990 July 1990</small>		

A gas in the sense of this Guideline is to be considered as “heavy” if the following criteria apply (see also Appendix A):

- the relative density excess of the gas at the place of release  $\Delta \rho_0/\rho_a$  amounts to more than 0.16,
- simultaneously, for instantaneous release, the source volume  $V_0$  amounts to more than  $0.1 \text{ m}^3$ , or, for continuous release, the source volume flow rate  $\dot{V}_0$  is larger than  $1 \cdot 10^{-3} \text{ m}^3/\text{s}$ .

If both criteria are not fulfilled simultaneously, the procedure described in Guideline VDI 3783 Part 1 is to be applied. The same holds if it can be reasonably excluded, on the basis of the source conditions, that the gas can disperse near the ground.

The following definitions hold:

$$\Delta \rho_0/\rho_a = (\rho_0 - \rho_a)/\rho_a$$

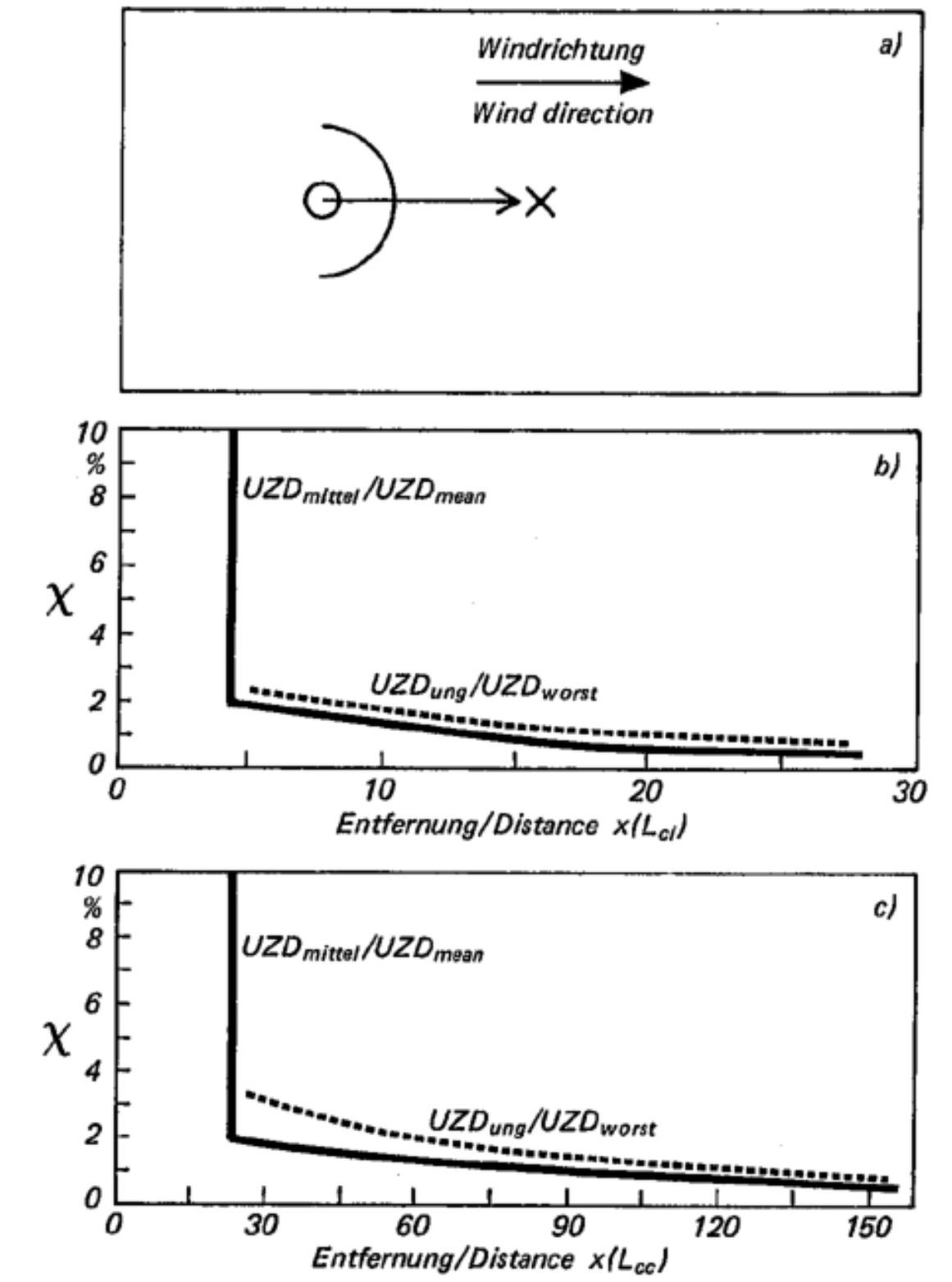
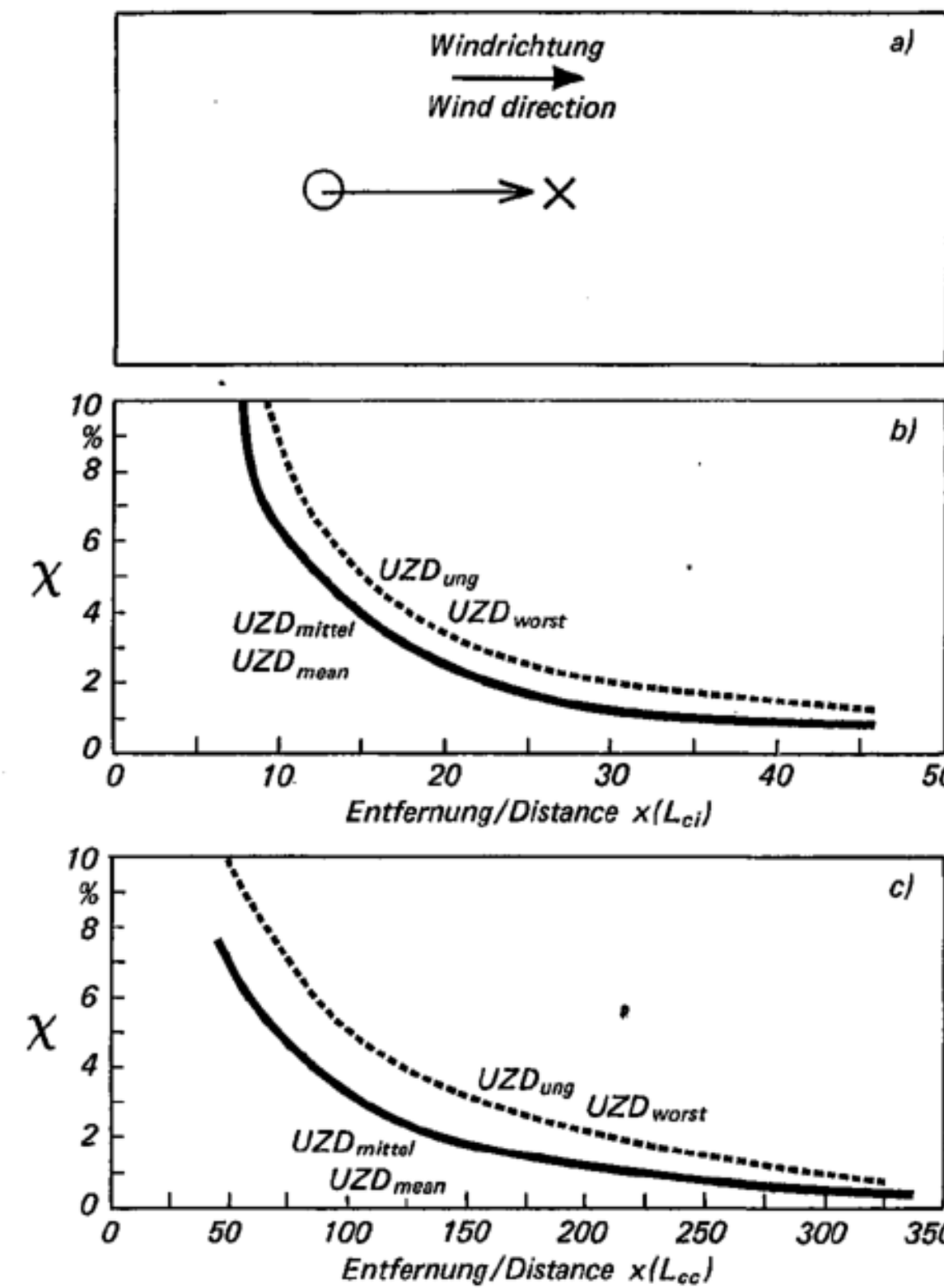
relative density difference of the gas at the source, with

$\rho_0$  density of the gas at the source according to Section 3.1 in  $\text{kg}/\text{m}^3$ . If the gas has been diluted with air before the release, the density of the gas mixture is to be used in divergence of Section 3.1.

$\rho_a$  density of the ambient air at source height in  $\text{kg}/\text{m}^3$  (It is recommended to calculate with  $\rho_a = 1.2 \text{ kg}/\text{m}^3$ .)

$V_0$  source volume of the gas according to Section 3.2 in  $\text{m}^3$

$\dot{V}_0$  source volume flow rate of the gas according to Section 3.2 in  $\text{m}^3/\text{s}$



<https://www.vdi.de/en/home/vdi-standards/details/vdi-3783-blatt-2-environmental-meteorology-dispersion-of-heavy-gas-emissions-by-accidental-releases-safety-study>

The normalized concentration  $\chi$  is defined as the ratio of the local volume concentration to the volume concentration at the source, and it is indicated in %. The distance from the source  $x$  is indicated in the characteristic length scales  $L_{ci}$  (for instantaneous release according to Section 3.3) resp.  $L_{cc}$  (for continuous release according to Section 3.3).

b) Continuous release (according to Section 3.3)  
 $L_{cc} = (\dot{V}_0^2/g_e)^{1/5}$  characteristic length scale in m



# Integral models

- Commercial software and/or freely-available integral models

- Arkansas University DEGADIS (also ALOHA) [www.epa.gov/scram/air-quality-dispersion-modeling-alternative-models#degadis](http://www.epa.gov/scram/air-quality-dispersion-modeling-alternative-models#degadis)
- CERC GASTAR [www.cerc.co.uk/environmental-software/GASTAR-model.html](http://www.cerc.co.uk/environmental-software/GASTAR-model.html)
- DNV PHAST [www.dnv.com/software/services/plant/consequence-analysis-phast](http://www.dnv.com/software/services/plant/consequence-analysis-phast)
- ESR DRIFT [www.esrtechnology.com/safety-risk/what-we-do/software/drift/](http://www.esrtechnology.com/safety-risk/what-we-do/software/drift/)
- JRC ADAM [adam.jrc.ec.europa.eu/en/adam/content](http://adam.jrc.ec.europa.eu/en/adam/content)
- LLNL SLAB [www.epa.gov/scram/air-quality-dispersion-modeling-alternative-models](http://www.epa.gov/scram/air-quality-dispersion-modeling-alternative-models)
- Shell HEGADAS [www.hgssystem.com](http://www.hgssystem.com)
- Shell FRED [www.gexcon.com/software/shell-fred/](http://www.gexcon.com/software/shell-fred/)
- TNO EFFECTS [www.gexcon.com/software/effects/](http://www.gexcon.com/software/effects/)

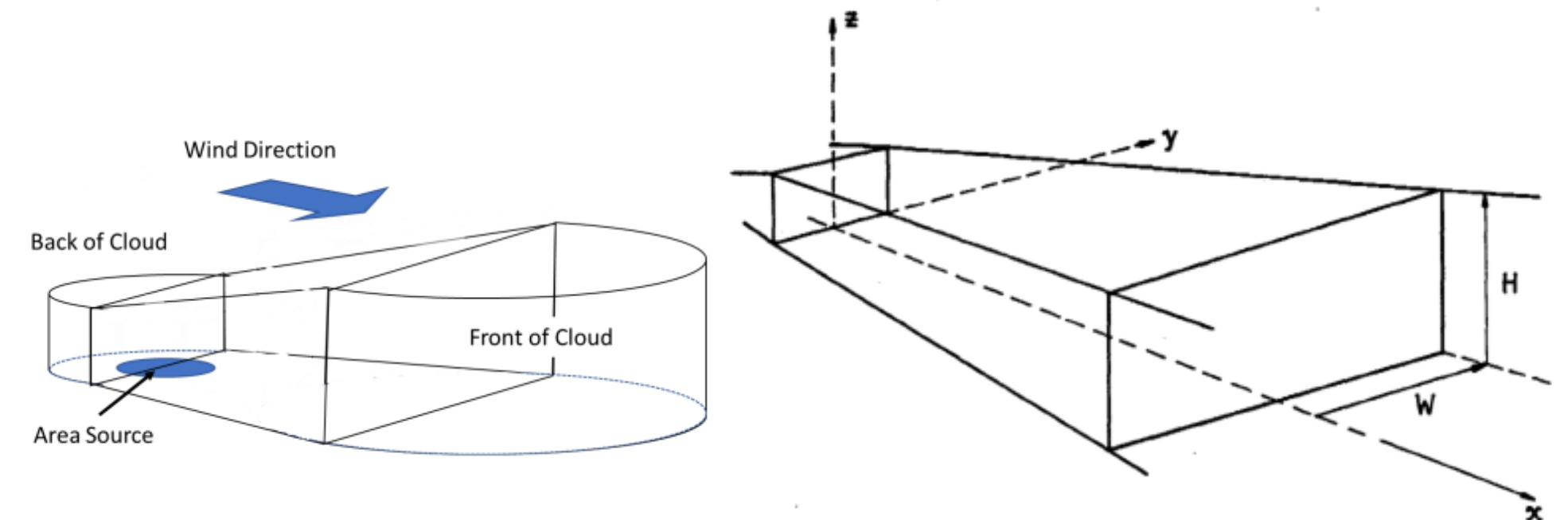


Figure 3. Schematic diagram of DRIFT's area source option

<https://doi.org/10.1016/j.atmosenv.2020.117717>

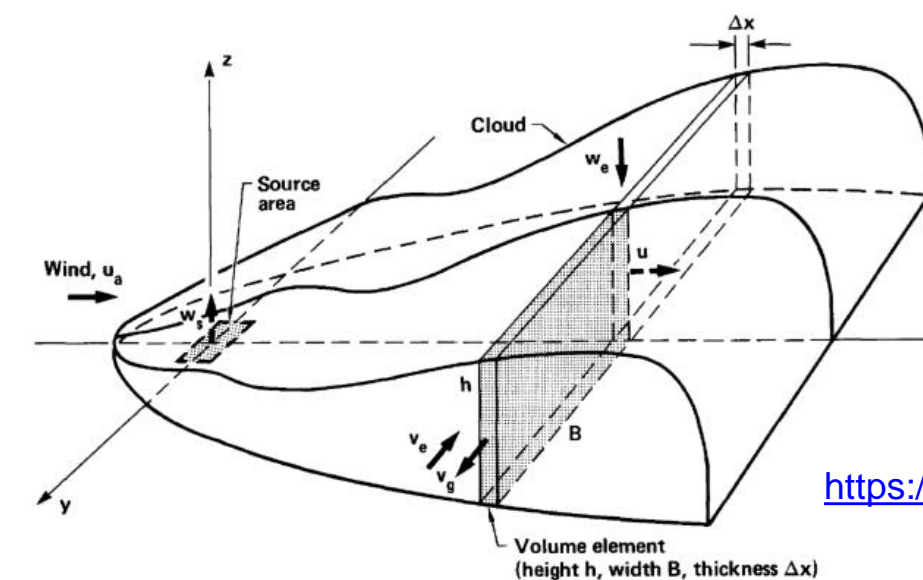


Figure 1. Depiction of a dispersing cloud of heavy gas and air as assumed by the SLAB model, so named because of the slab-shaped volume element.

<https://www.osti.gov/biblio/6271522>

FIG. 3 A REPRESENTATION OF THE CLOUD

[https://admlc.com/wp-content/uploads/2023/09/webber\\_jones\\_tickle\\_wren\\_1992\\_implementation\\_drift\\_model\\_continuous\\_releases\\_srd\\_r587.pdf](https://admlc.com/wp-content/uploads/2023/09/webber_jones_tickle_wren_1992_implementation_drift_model_continuous_releases_srd_r587.pdf)

- Future talk to Met Office/HSE by Gemma Tickle (DRIFT developer) on integral models

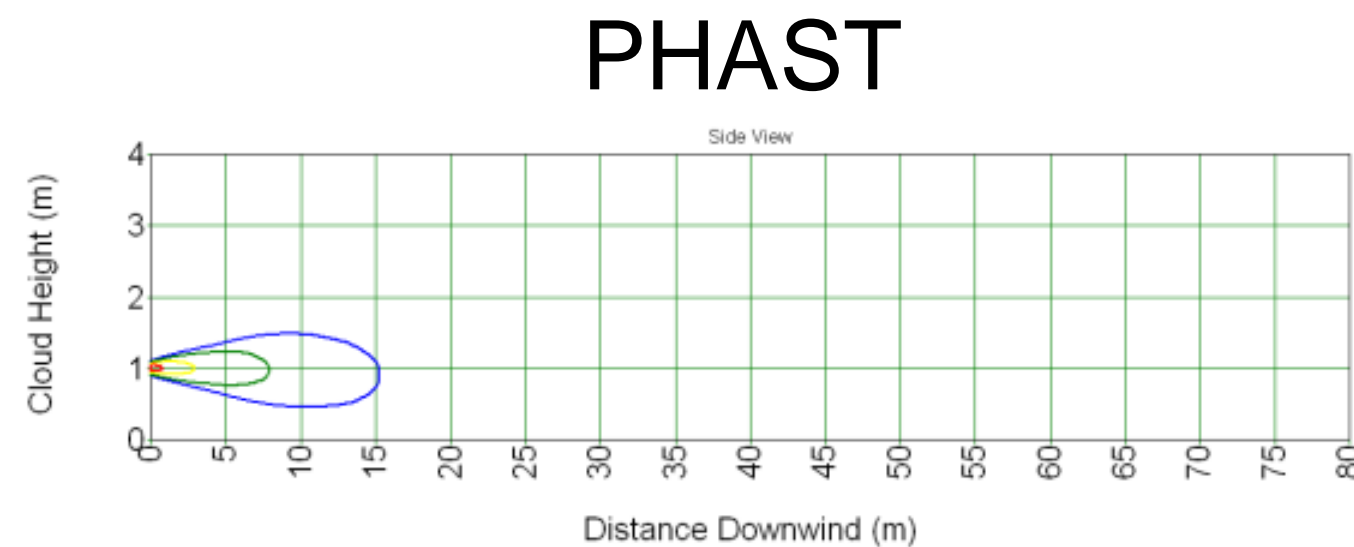


# Integral models

- Examples of integral model predictions

Orifice Diameter

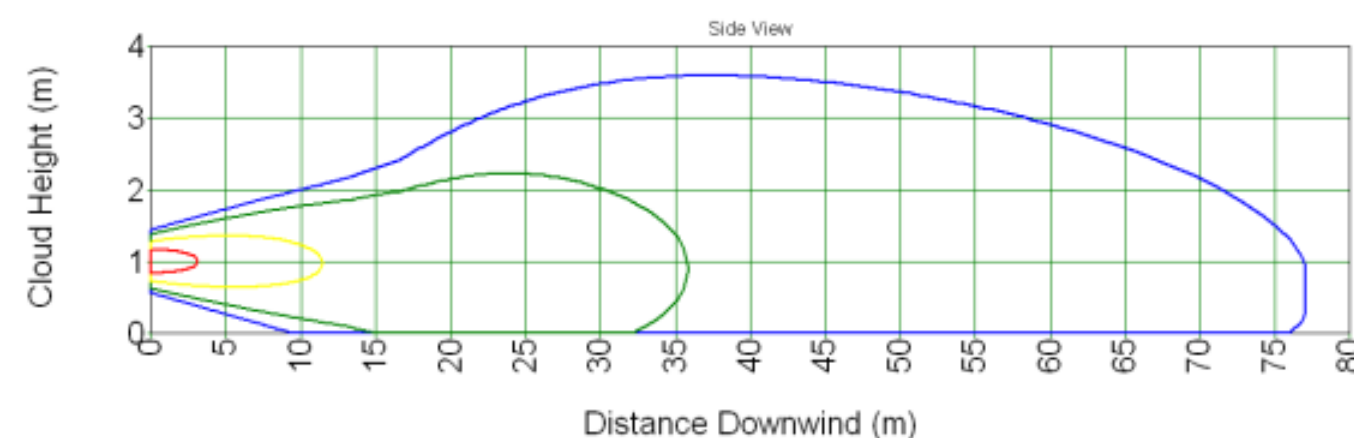
½ inch



1 inch



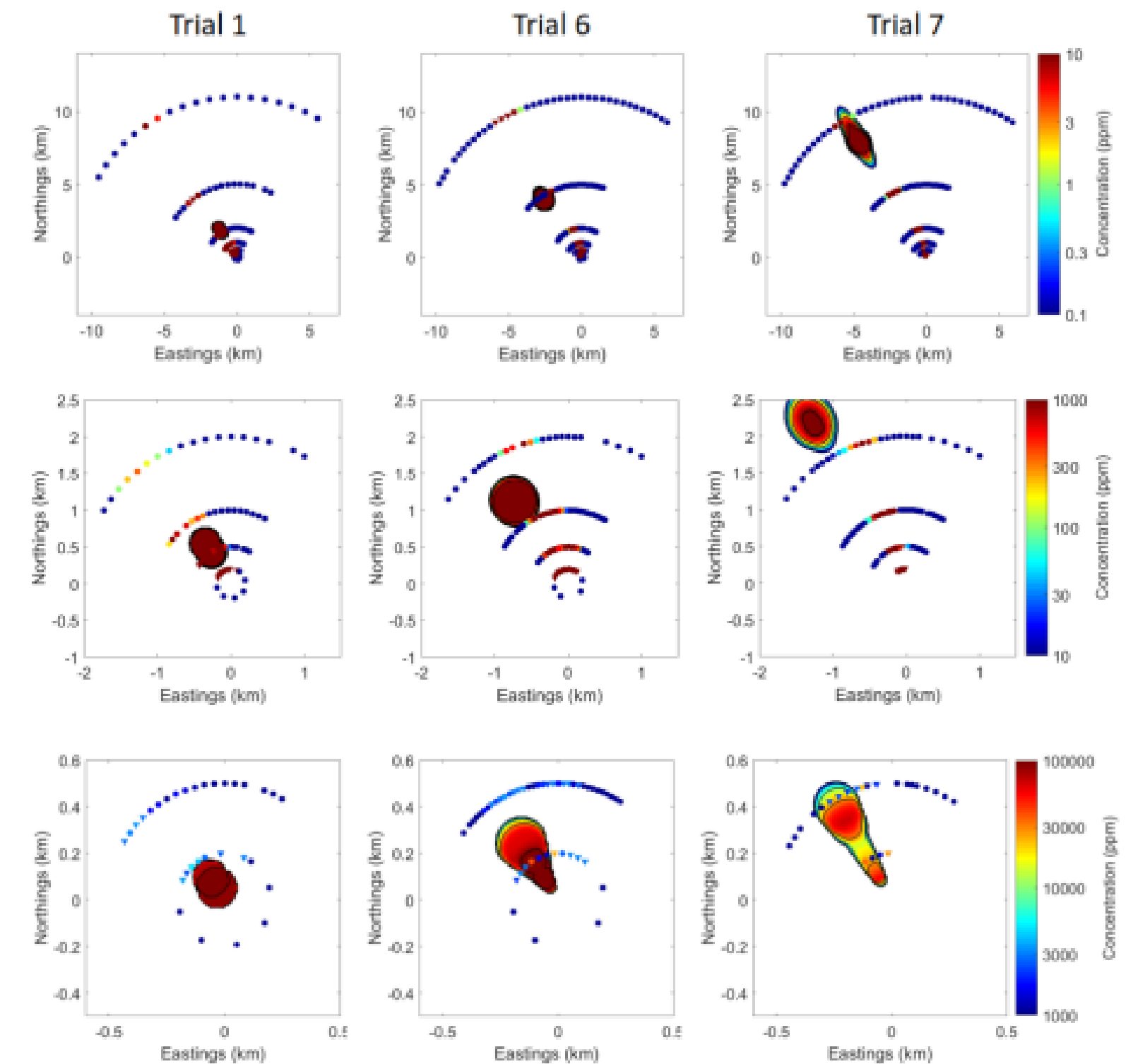
2 inch



## PHAST

[http://gant.org.uk/research/Gant\\_LP2013a.pdf](http://gant.org.uk/research/Gant_LP2013a.pdf)

## DRIFT



**Figure 10** DRIFT1 predicted concentration contours for Trials 1, 6 and 7, at three locations: near, mid and far-field (shown in the bottom, middle and top plots, respectively). Coloured symbols show measured maximum concentrations (over all time), whereas contours show a snapshot of the predicted concentration at the time intervals of 120 s, 600 s and 1800 s in the near, mid and far-field, respectively. Triangular symbols indicate the sensor saturated, whereas round symbols indicate the sensors were unaffected by saturation issues. Both the contours and symbols use the same colour scales. Predicted concentrations below lower limit of the colour scale (e.g. 1,000 ppm in the near-field plots) are not shown, i.e. contour limits are clipped to this lower bound so that the background appears white, not blue.

<https://doi.org/10.1016/j.atmosenv.2020.117717>



# Integral models

## ■ Capabilities

- Fast to compute: typically seconds or minutes on a standard laptop
- Different sources: vessels, pipelines, small holes, catastrophic ruptures
- Single and two-phase releases (assuming homogenous equilibrium)
- Liquid rainout and pool evaporation
- Initial jet dispersion and later transition to passive plume (in addition to dense gas dispersion)
- Different release directions relative to wind direction (up/down/sideways)
- Condensation of atmospheric moisture and latent heat effects
- Complex reactions, e.g., oligomerization of hydrogen fluoride, water-reactive substances

Only some integral models have these complex features

## ■ Limitations

- Flat terrain (or continuous uniform slopes) with uniform roughness
- Steady atmospheric conditions (single wind profile and atmospheric stability)



# Gaussian puff, Lagrangian and Röckle models

- ARGOS <https://pdc-argos.com/>
  - AUSTAL <http://austal.de>
  - FOI PUMA and LPELLO <https://doi.org/10.1016/j.atmosenv.2020.117521>
  - LANL QUIC <https://www.lanl.gov/projects/quic/>
  - Riskaware UDM <https://www.riskaware.co.uk/wp-content/uploads/HASP-Suite-UDM.pdf>
  - SCIPUFF (also HPAC) <https://github.com/epri-dev/SCICHEM/releases>
  - SUEZ-ARIA Micro SWIFT/SPRAY
- Compute times: typically minutes to hours
  - Capable of simulating buildings, obstacles, and (in principle) complex terrain
  - Some models (e.g., HPAC) have a range of in-built complex source models

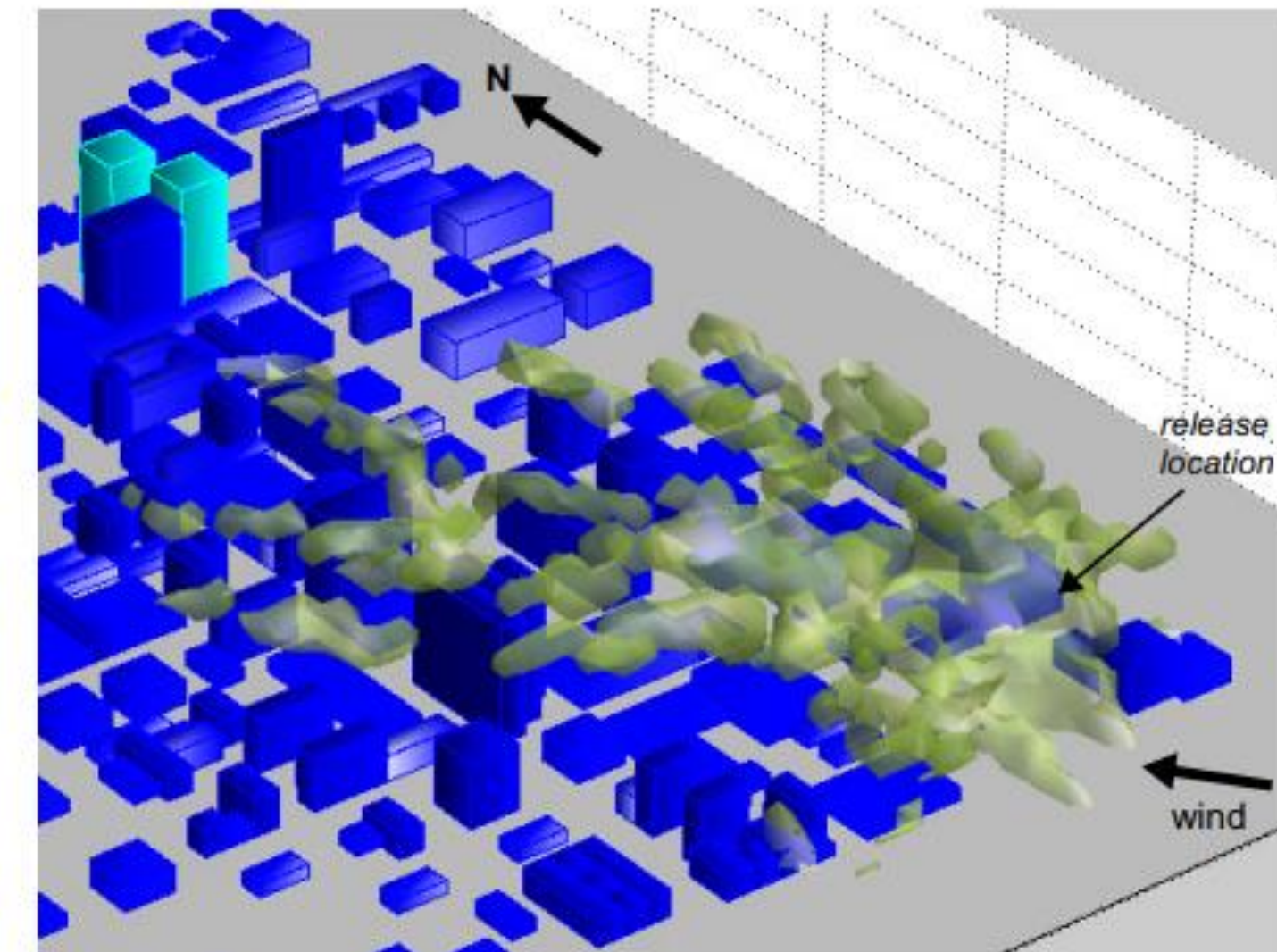


Figure 2. QUIC-PLUME simulation of CB agent transport and dispersion in downtown Salt Lake City. The agent cloud is quickly lofted into the air due to the presence of tall buildings. The inflow wind is from the southeast.

[https://www.lanl.gov/projects/quic/open\\_files/QUIC\\_factsheet.pdf](https://www.lanl.gov/projects/quic/open_files/QUIC_factsheet.pdf)

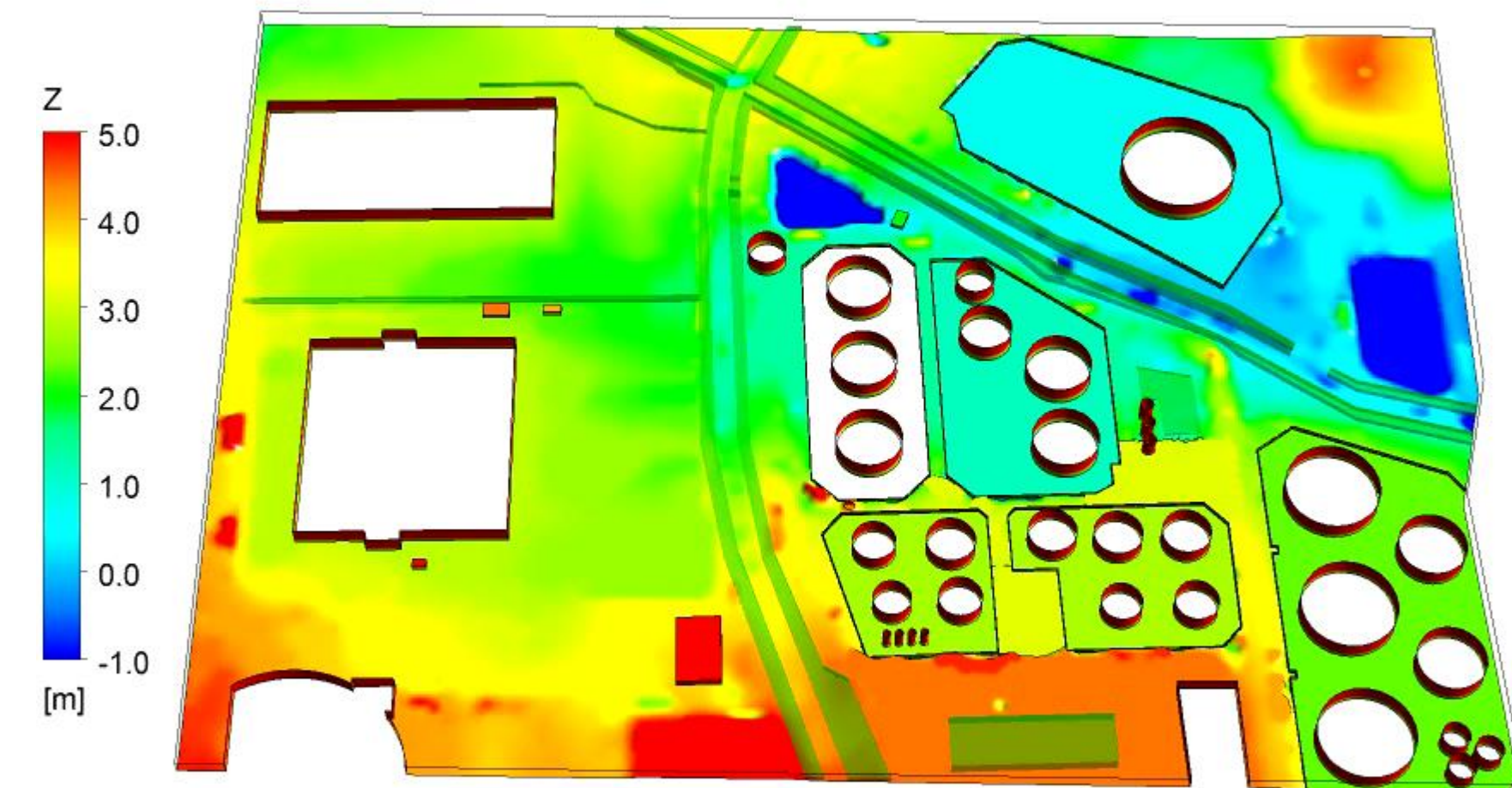


# Computational Fluid Dynamics (CFD)

- ANSYS Fluent/CFX <https://www.ansys.com/>
- Demokritos ADREA-HF  
<https://doi.org/10.1016/j.ijhydene.2010.01.002>
- DNV KFX <https://www.dnv.com/services/cfd-simulation-kfx-110662>
- EDF Code-Saturne <https://www.code-saturne.org/>
- OpenFOAM <https://www.openfoam.com/>
- Gexcon FLACS <https://www.gexcon.com/software/flacs-cfd/>
- Siemens Star-CCM+ <https://plm.sw.siemens.com/en-US/simcenter/fluids-thermal-simulation/star-ccm/>

Time = 0 [mins] 0 [sec]

Isosurface: Petrol Vapour Molar Fraction 1.6%



- Computing times: hours to days on high-performance computers
- Complex physics: evaporation, condensation, two-phase flows, pool evaporation etc.
- Flexible geometry: terrain, buildings, obstacles
- Atmospheric boundary layers are challenging to model in CFD (see <https://doi.org/10.1504/IJEP.2018.093026>)



# Shallow layer, lattice-Boltzmann, SPH etc.

- Shallow layer models
  - TWODEE
  - SPLOT
  - DISPLAY
  - KLAM (katabatic flows) <https://admlc.com/events/>



Smoothed Particle Hydrodynamics (SPH)

<https://www.spheric-sph.org/>

Physics of Fluids

ARTICLE

[scitation.org/journal/phf](https://scitation.org/journal/phf)

## Graphics processing unit accelerated lattice Boltzmann method simulations of dilute gravity currents

Cite as: Phys. Fluids **34**, 046602 (2022); doi: 10.1063/5.0082959

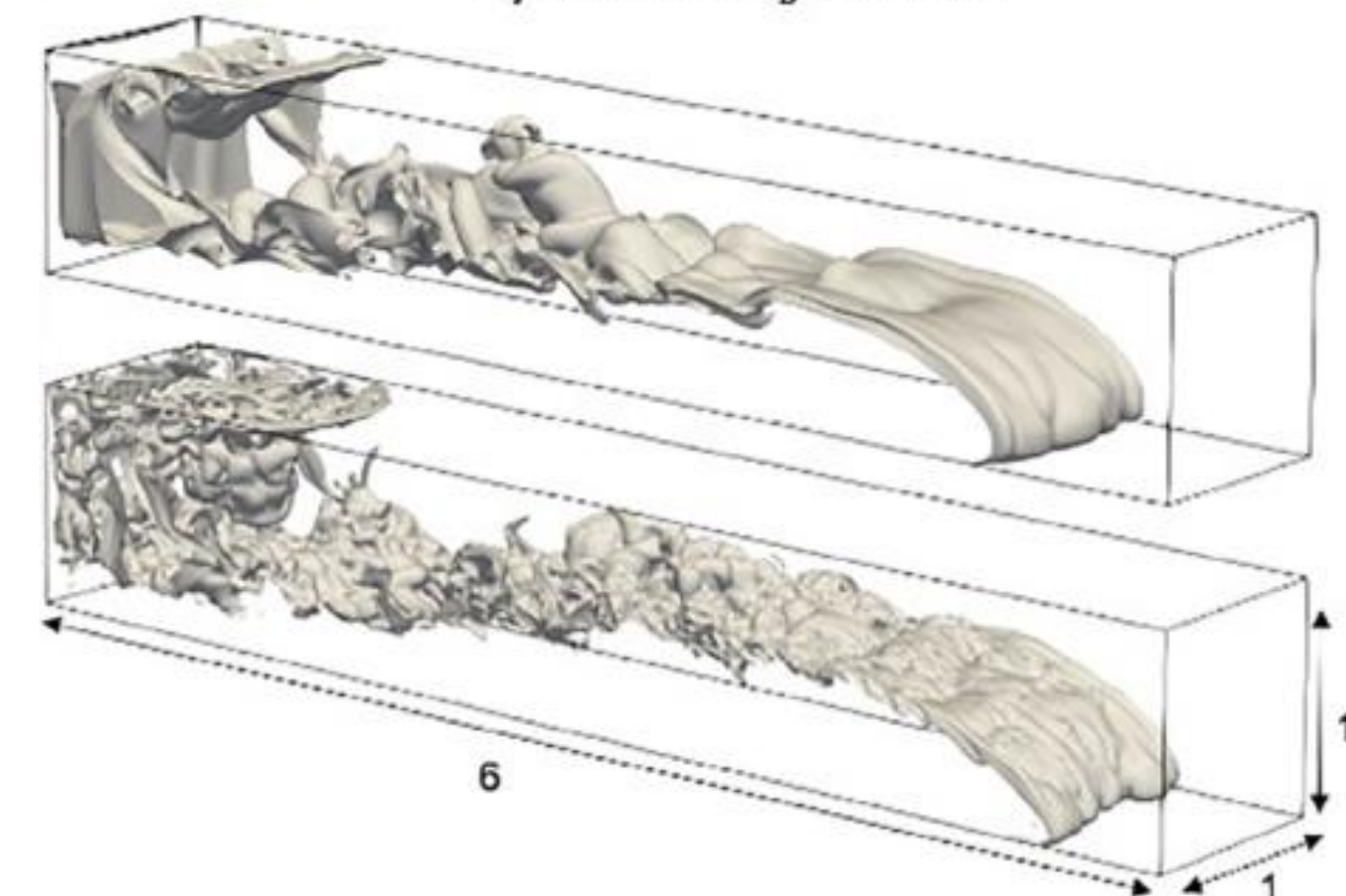
Submitted: 20 December 2021 · Accepted: 7 February 2022 ·

Published Online: 7 April 2022



Damilola Adekanye,<sup>1,a)</sup> Amirul Khan,<sup>2</sup> Alan Burns,<sup>3</sup> William McCaffrey,<sup>4</sup> Martin Geier,<sup>5</sup> Martin Schönherr,<sup>5</sup> and Robert Dorrell<sup>6</sup>

d) Case 8 -  $Re_b = 30000$ :





# Summary of results from the Jack Rabbit III international model inter-comparison exercise on Desert Tortoise and FLADIS

Simon Gant<sup>1</sup>, Joseph Chang<sup>2</sup>, Sun McMasters<sup>3</sup>, Ray Jablonski<sup>3</sup>, Helen Mearns<sup>3</sup>, Shannon Fox<sup>3</sup>, Ron Meris<sup>4</sup>, Scott Bradley<sup>4</sup>, Sean Miner<sup>4</sup>, Matthew King<sup>4</sup>, Steven Hanna<sup>5</sup>, Thomas Mazzola<sup>6</sup>, Tom Spicer<sup>7</sup>, Rory Hetherington<sup>1</sup>, Alison McGillivray<sup>1</sup>, Adrian Kelsey<sup>1</sup>, Harvey Tucker<sup>1</sup>, Graham Tickle<sup>8</sup>, Oscar Björnham<sup>9</sup>, Bertrand Carissimo<sup>10</sup>, Luciano Fabbri<sup>11</sup>, Maureen Wood<sup>11</sup>, Karim Habib<sup>12</sup>, Mike Harper<sup>13</sup>, Frank Hart<sup>13</sup>, Thomas Vik<sup>14</sup>, Anders Helgeland<sup>14</sup>, Joel Howard<sup>15</sup>, Veronica Bowman<sup>15</sup>, Daniel Silk<sup>15</sup>, Lorenzo Mauri<sup>16</sup>, Shona Mackie<sup>16</sup>, Andreas Mack<sup>16</sup>, Jean-Marc Lacomme<sup>17</sup>, Stephen Puttick<sup>18</sup>, Adeel Ibrahim<sup>18</sup>, Derek Miller<sup>19</sup>, Seshu Dharmavaram<sup>19</sup>, Amy Shen<sup>19</sup>, Alyssa Cunningham<sup>20</sup>, Desiree Beverley<sup>20</sup>, Matthew O'Neal<sup>20</sup>, Laurent Verdier<sup>21</sup>, Stéphane Burkhart<sup>21</sup>, Chris Dixon<sup>22</sup>

<sup>1</sup>Health and Safety Executive (HSE), <sup>2</sup>RAND Corporation, <sup>3</sup>Chemical Security Analysis Center (CSAC), Department of Homeland Security (DHS), <sup>4</sup>Defense Threat Reduction Agency (DTRA), <sup>5</sup>Hanna Consultants, Inc., <sup>6</sup>Systems Planning and Analysis, Inc. (SPA), <sup>7</sup>University of Arkansas, <sup>8</sup>GT Science and Software, <sup>9</sup>Swedish Defence Research Agency (FOI), <sup>10</sup>EDF/Ecole des Ponts, <sup>11</sup>European Joint Research Centre (JRC), <sup>12</sup>Bundesanstalt für Materialforschung und -prüfung (BAM), <sup>13</sup>DNV, Stockport, <sup>14</sup>Norwegian Defence Research Establishment (FFI), <sup>15</sup>Defence Science and Technology Laboratory (DSTL), <sup>16</sup>Gexcon, <sup>17</sup>Institut National de l'Environnement Industriel et des Risques (INERIS), <sup>18</sup>Syngenta, <sup>19</sup>Air Products, <sup>20</sup>Naval Surface Warfare Center (NSWC), <sup>21</sup>Direction Générale de l'Armement (DGA), <sup>22</sup>Shell

*21st International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*  
*27-30 September 2022*



# Methodology

- Simulate 3 trials each from the Desert Tortoise and FLADIS pressure-liquefied ammonia field trials
- Desert Tortoise
  - Tests conducted in 1983 at DOE Nevada Test Site
  - Release rates of 81 – 133 kg/s
  - 10 – 41 tonnes of ammonia released
  - Dispersion measurements at 100 m and 800 m
  - Largest tests to date on ammonia
- FLADIS
  - Tests conducted in 1993-4 at Landskrona, Sweden
  - Release rates of 0.25 – 0.55 kg/s
  - Dispersion measurements at 20 m, 70 m and 240 m (transition from dense to passive dispersion)

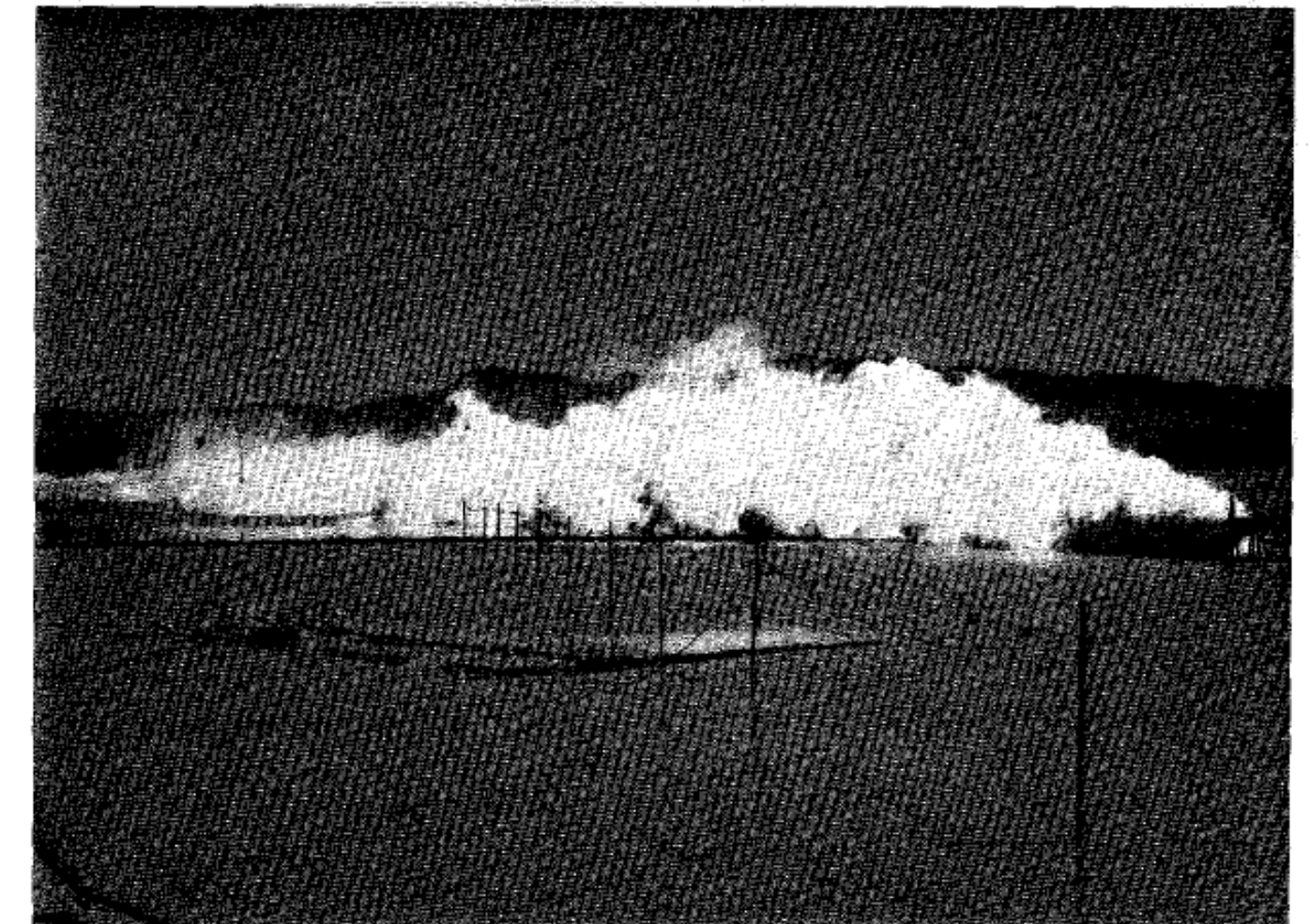


Fig. 15. Desert Tortoise 2 (upwind wide angle camera) Time = 230s. Lawrence Livermore National Laboratory



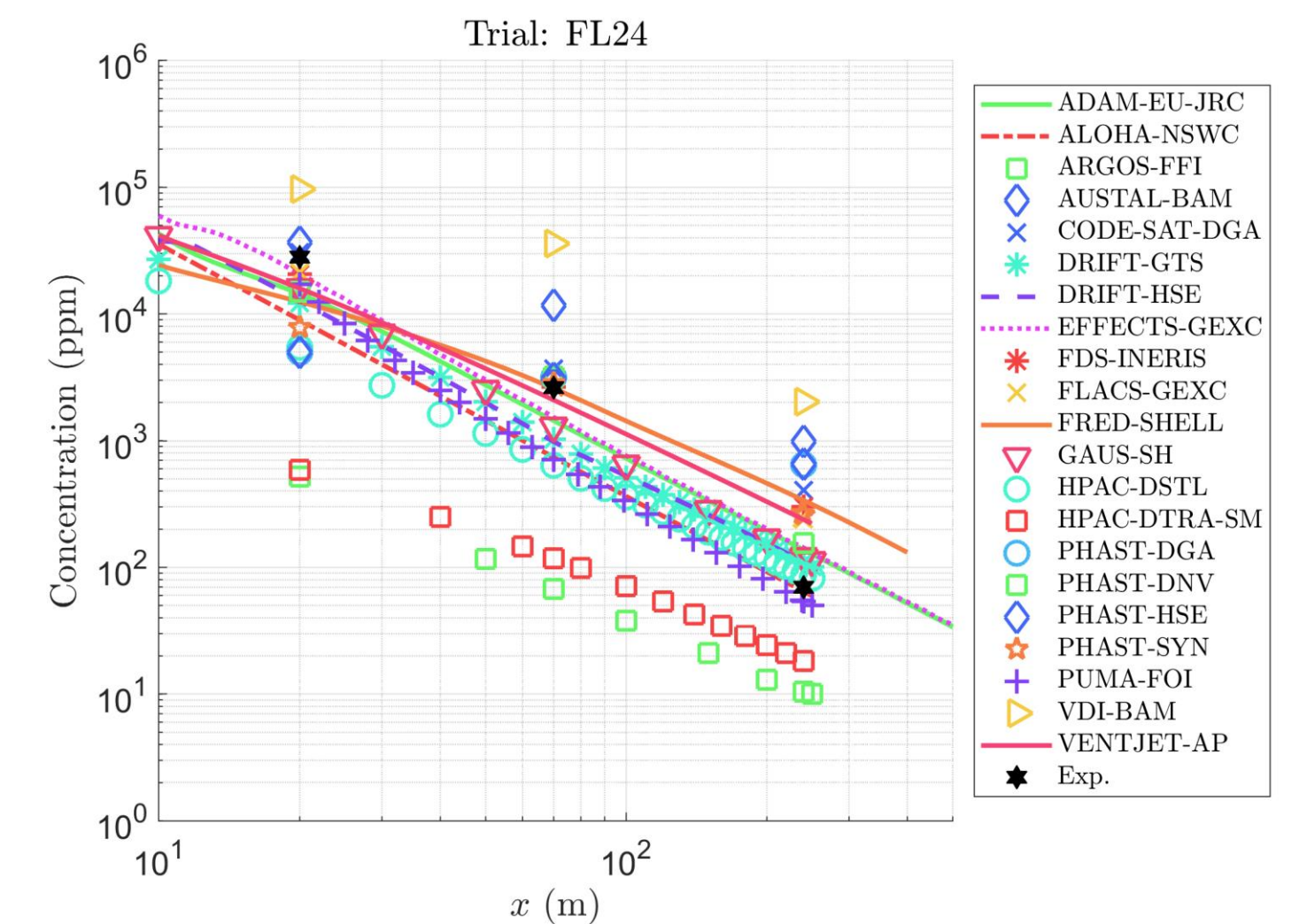
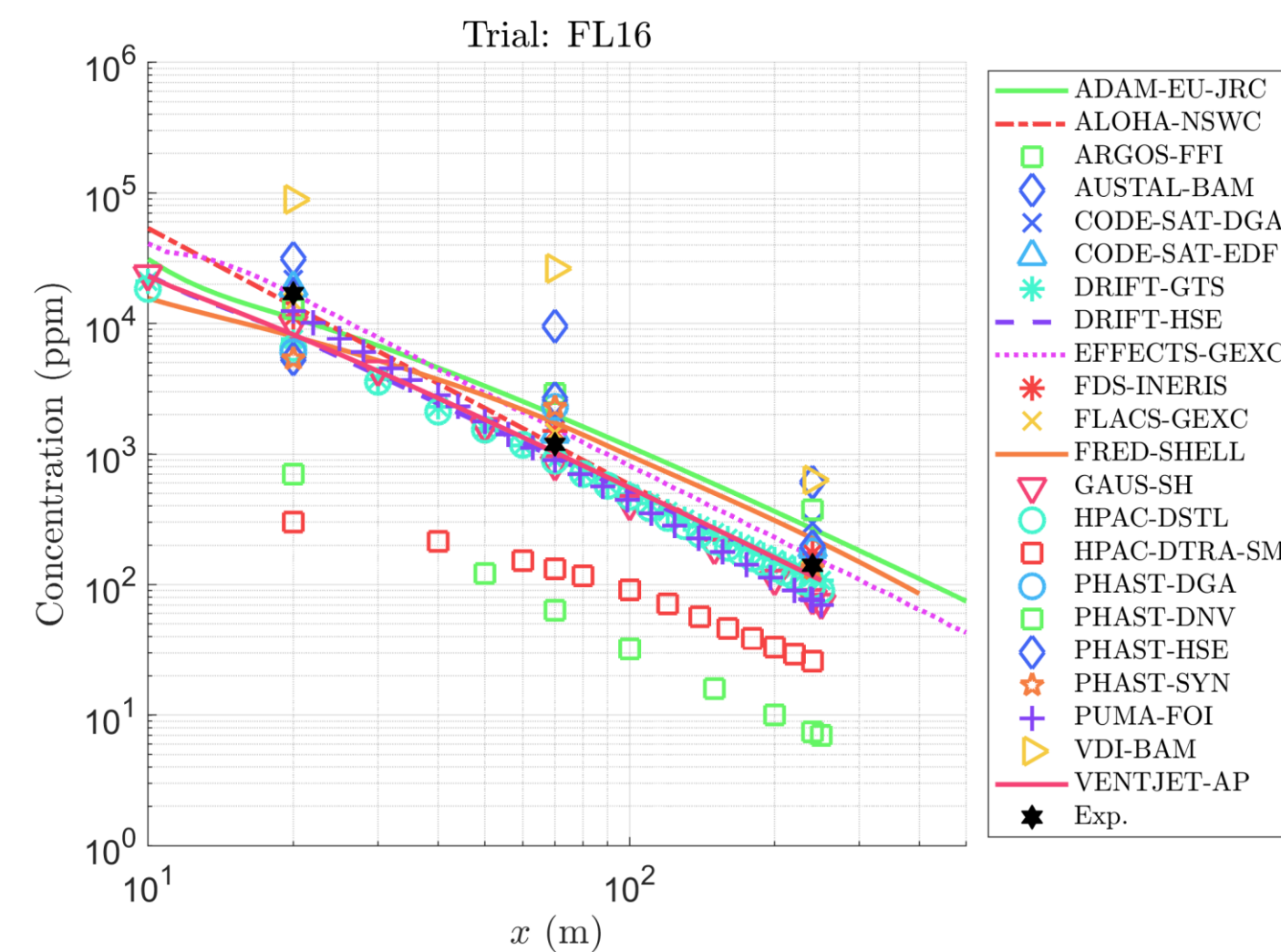
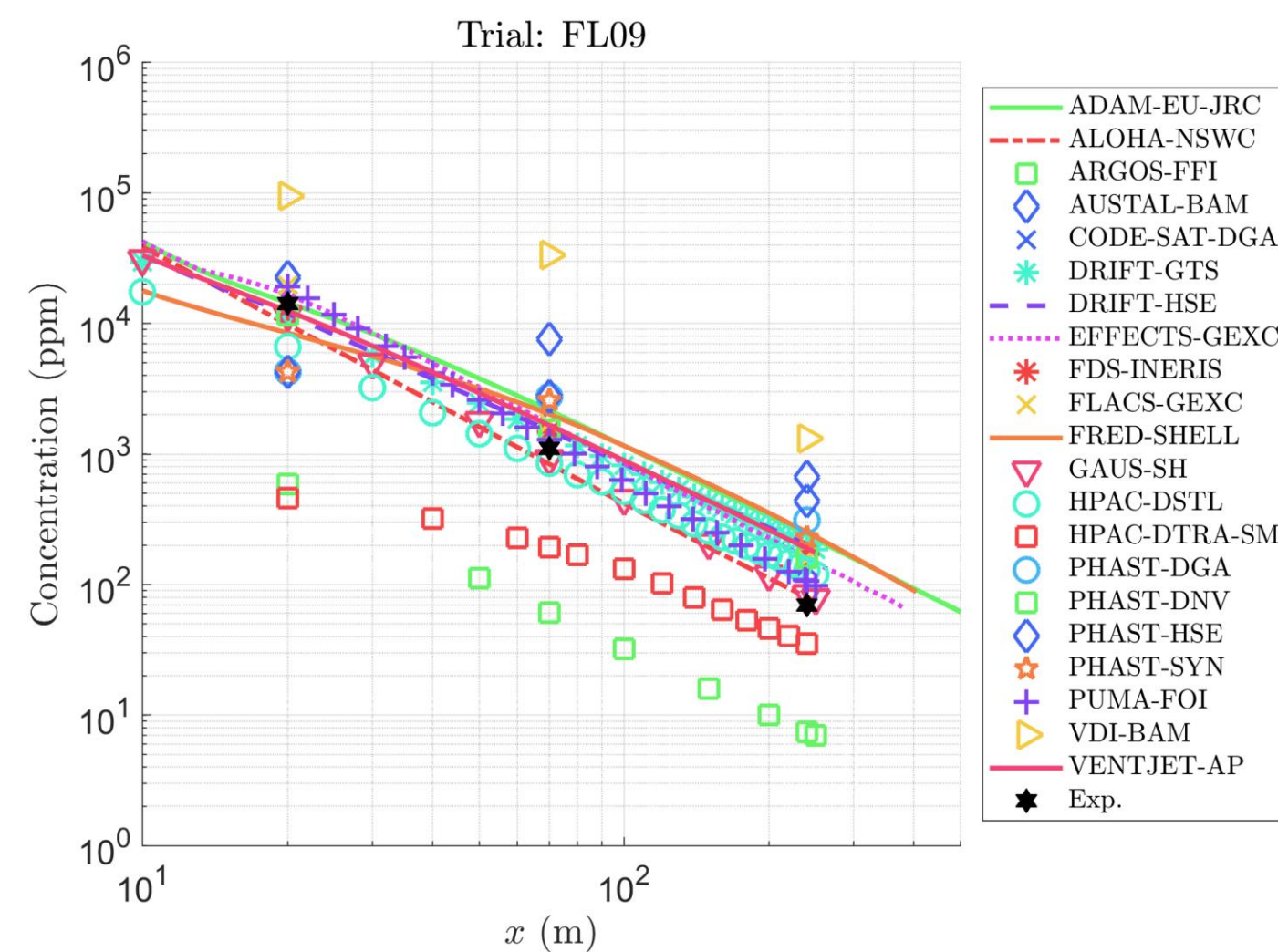
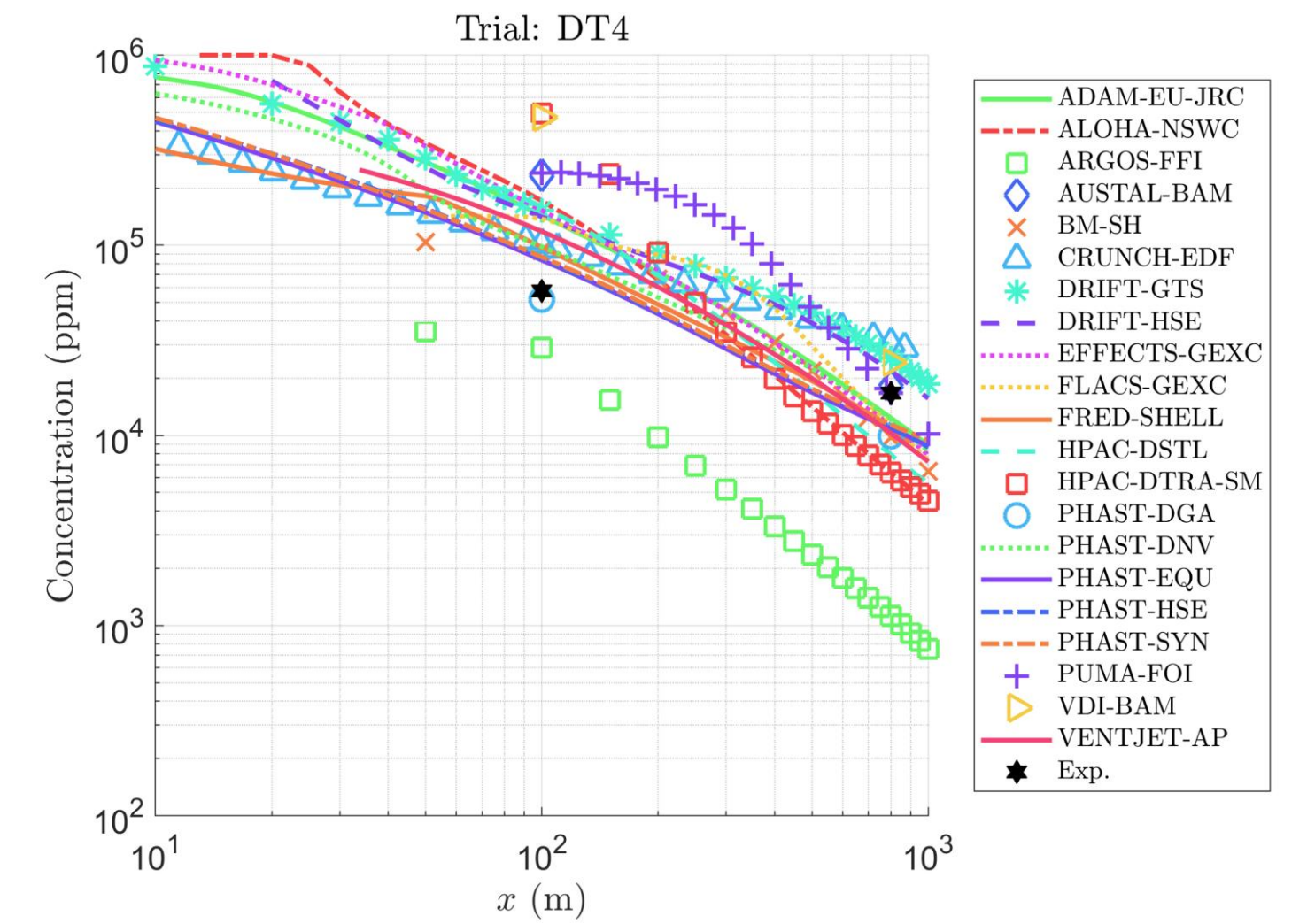
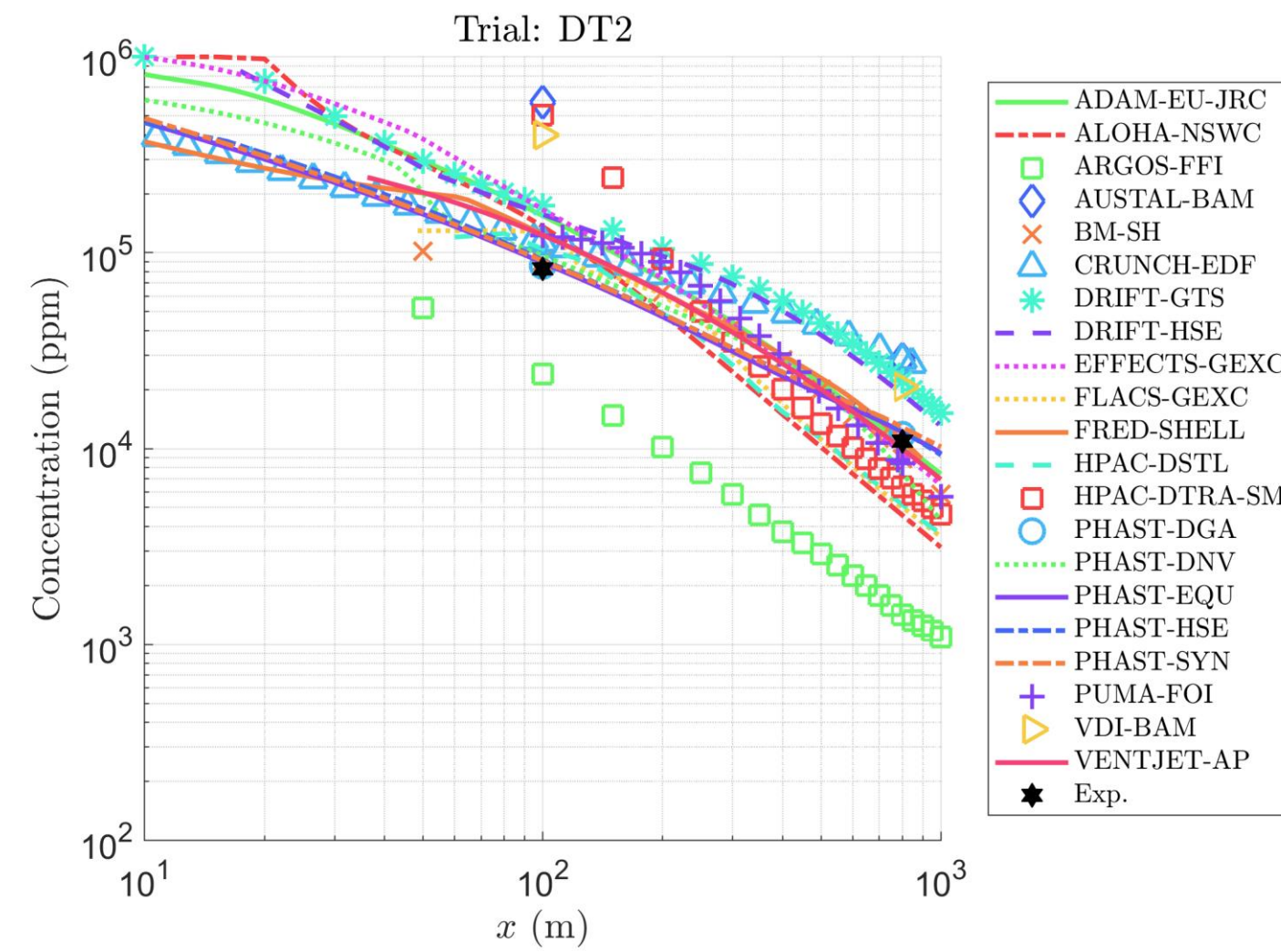
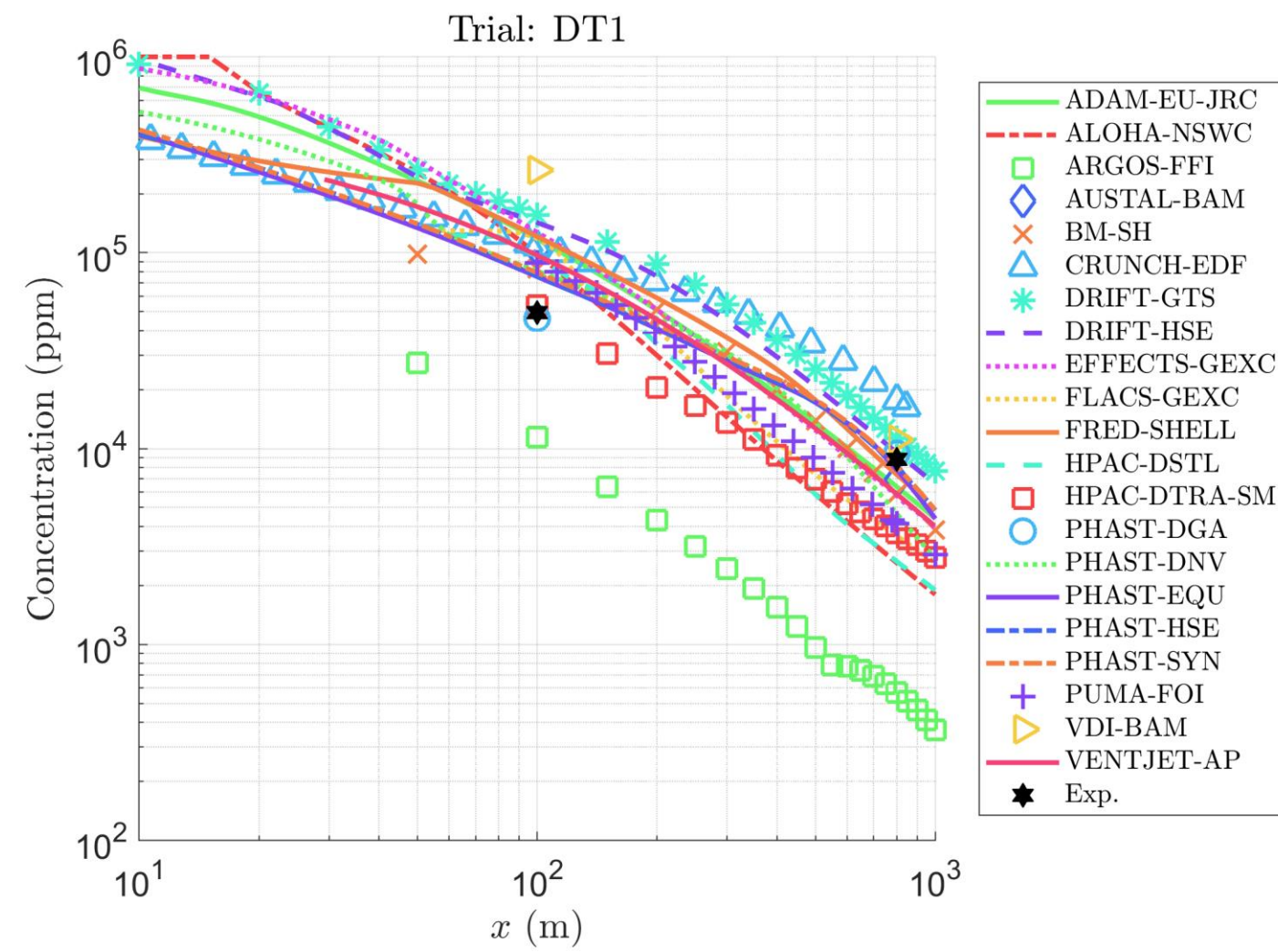


# Participants in the JR111 initial modeling exercise

#	Organization	Model	Model Type				Desert Tortoise			FLADIS		
			Empirical nomogram/ Gaussian plume	Integral	Gaussian Puff/ Lagrangian	CFD	1	2	4	9	16	24
1	Air Products, USA	VentJet										
2	BAM, Germany	AUSTAL										
3		VDI										
4	DGA, France	PHAST v8.6										
5		Code-Saturne v6.0										
6	DNV, UK	PHAST v8.61										
7	DSTL, UK	HPAC v6.5										
8	DTRA, ABQ, USA	HPAC v6.7										
9	DTRA, Fort Belvoir, USA	HPAC										
10	EDF/Ecole des Ponts, France	Code-Saturne v7.0										
11		Crunch v3.1										
12	Equinor, Norway	PHAST v8.6										
13	FFI, Norway	ARGOS v9.10										
14	FOI, Sweden	PUMA										
15	Gexcon, Netherlands	EFFECTS v11.4										
16	Gexcon, Norway	FLACS										
17	GT Science & Software	DRIFT v3.7.19										
18	Hanna Consultants, USA	Britter & McQuaid WB										
19		Gaussian plume model										
20	HSE, UK	DRIFT v3.7.12										
21		PHAST v8.4										
22	INERIS, France	FDS v6.7										
23	JRC, Italy	ADAM v3.0										
24	NSWC, USA	RAILCAR-ALOHA										
25	Shell, UK	FRED 2022										
26	Syngenta, UK	PHAST v8.61										



# All model results





# Summary of dense gas experiments by Rachel Batt (2021)

Name  
 Substance  
 Flammable  
 Toxic/health  
 Field  
 Wind tunnel  
 Land  
 Water  
 Instantaneous  
 Continuous  
 Cryogenic  
 Pressurised  
 Liquid jet  
 Gas source  
 Flashing  
 Low momentum  
 Reactive  
 Complex source

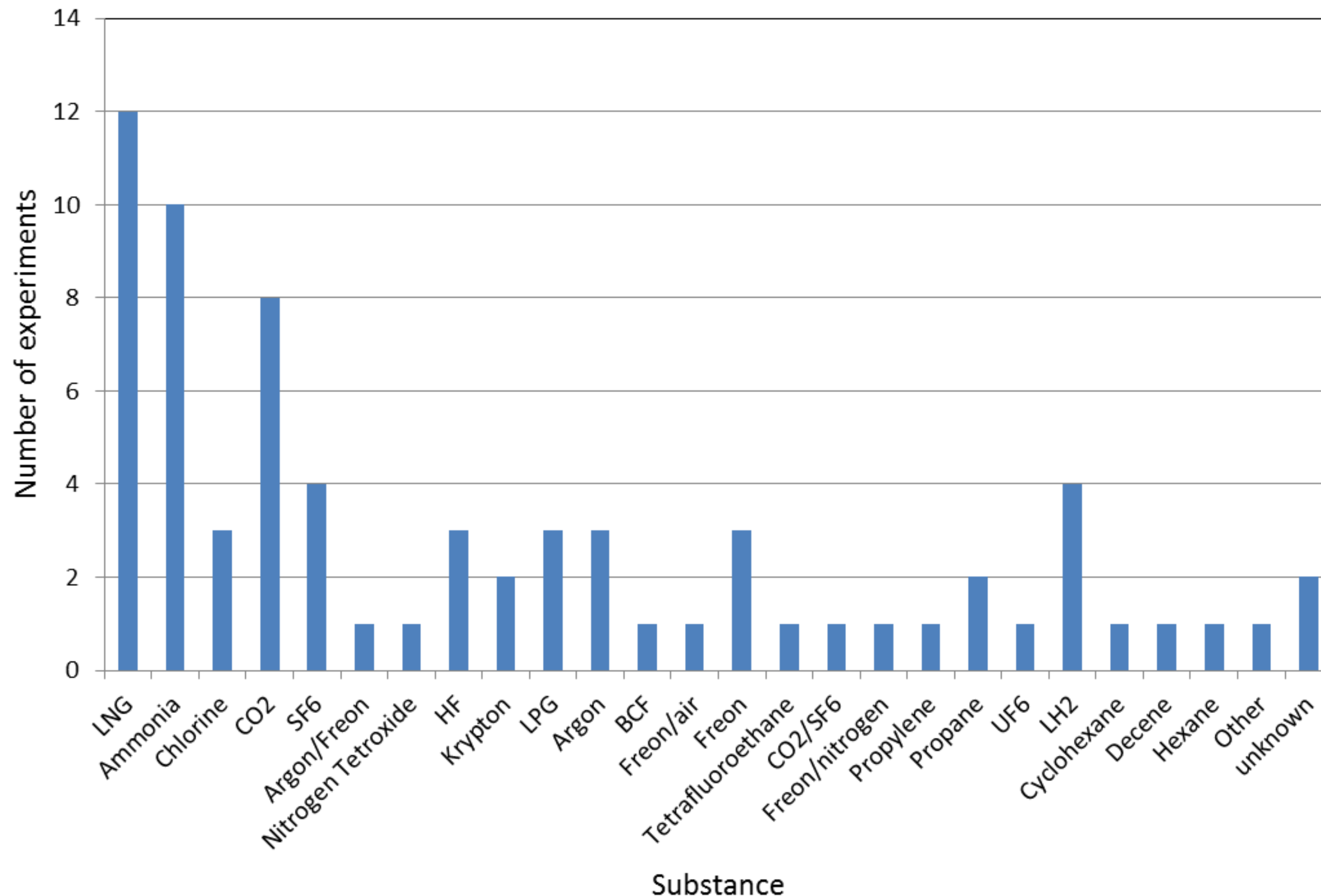
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
1																													
2		Substance	Flammab	Toxic	Field	Wind tun	Land	Water	Inst	Cont	Cryogenic	Pressuris	Liquid jet	Elevated	Liquid po	Gas sourc	Flashing	Low mom	Reactive	Complex	Unobstru	Obstructi	Topograp	Potential	Nil/low w	Concentr	Ingress	Mitigatio	Uncerta
3	AGA	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
4	API/Esso	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
5	Atkinson	Hexane, v	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
6	Avocet	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
7	BA Hamb	SF6	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
8	BA TNO	SF6	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
9	BMT	Argon/Freon	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
10	Bureau of	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
11	Burro	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
12	CHRC	CO2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
13	China Lak	Argon, Freon-12	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
14	COOLTRAN	CO2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
15	Coyote	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
16	Desert To	Ammonia	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
17	Eagle	Nitrogen	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
18	Ecole des	Ammonia	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
19	Egami et	CO2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
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21	ENFLO 20	CO2, krypton	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
22	Enflo 200	3% propane in CO2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
23	Falcon	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
24	FLADIS	Ammonia	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
25	FLIE	LPG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
26	Gadila	LNG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
27	Goldfish	HF	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
28	GRADE	LPG	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
29	Guldemo	Argon	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
30	Hall and	BCF, argon	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
31	Hoot et a	Freon/air mix	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
32	HSE 1985	CO2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
33	HSE 2012	LH2	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
34	ICHMAP	HF	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
35	Imperial	Ammonia	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
36	INERIS	Ammonia	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
37	Jack Rabb	Chlorine	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
38	Jack Rabb	Chlorine	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.	.

Unobstructed  
 Obstructed  
 Topography  
 Potential  
 porosity effects  
 Nil/ low wind/  
 stably stratified  
 Concentration  
 data  
 Ingress  
 Mitigation  
 Uncertainties  
 Previous model  
 validation  
 Potential model  
 validation  
 Reference

Excel spreadsheet available here: <https://admlc.com/publications/>



# Substances used in experiments



Top five substances in exps:

- Liquefied Natural Gas (LNG)
- Ammonia
- Carbon dioxide (CO<sub>2</sub>)
- Sulphur hexafluoride (SF<sub>6</sub>)
- Liquid hydrogen (LH<sub>2</sub>)

Top five substances in dense-gas incidents worldwide:

- Chlorine
- Ammonia
- Hydrogen sulphide
- LPG
- CO<sub>2</sub>, propane and gasoline



# Dense gas dispersion datasets

- Modelers Data Archive (MDA)
  - run by Joe Chang and Steve Hanna

## Data Sets Included in MDA

- |   |   |
|---|---|
| <ol style="list-style-type: none"> <li>1. Dense Gas MDA (including Burro, Coyote, Desert Tortoise, Goldfish, Lyme Bay, Maplin Sands, and Thorney Island)</li> <li>2. Prairie Grass</li> <li>3. Hanford Kr<sup>85</sup></li> <li>4. Ocean Breeze</li> <li>5. Dry Gulch</li> <li>6. Green Glow</li> <li>7. Kit Fox</li> <li>8. EPA CO<sub>2</sub></li> <li>9. DSWA Phase I</li> <li>10. DP26 (Dipole Pride 26)</li> <li>11. OLAD (Overland Alongwind Dispersion)</li> <li>12. MVP (Model Validation Program)</li> <li>13. Ventura</li> <li>14. Pismo Beach</li> <li>15. Cameron</li> <li>16. Carpinteria</li> <li>17. LROD (Long-Range Overwater Diffusion)</li> <li>18. MADONA (Meteorology And Diffusion Over Non-Uniform Areas)</li> <li>19. ACURATE (Atlantic Coast Unique Regional Atmospheric Tracer Experiment)</li> <li>20. ANATEX (Across North America Tracer Experiment)</li> <li>21. METREX (Metropolitan Tracer Experiment)</li> <li>22. CAPTEX (Cross Appalachian Tracer Experiment)</li> <li>23. ETEX (European Tracer Experiment)</li> <li>24. INEL74</li> <li>25. OKC80</li> <li>26. Birmingham</li> </ol> | <ol style="list-style-type: none"> <li>27. Urban 2000 (Salt Lake City)</li> <li>28. Joint Urban 2003 (Oklahoma City)*</li> <li>29. Madison Square Garden 2005*</li> <li>30. Midtown Manhattan 2005*</li> <li>31. MUST (Mock Urban Setting Test)</li> <li>32. EMU (Evaluation of Model Uncertainty)</li> <li>33. DPG Barrel</li> <li>34. LA 2001</li> <li>35. Barrio Logan (San Diego)</li> <li>36. Porton Down 1977</li> <li>37. Macdonald (water tunnel)</li> <li>38. SMEDIS (Scientific Model Evaluation of Dense Gas Dispersion Models)</li> <li>39. TRAPOS (Optimization of Modeling Methods for Traffic Pollution in Streets)</li> <li>40. REDIPHEM (Review and Dissemination of Physical Effects Models)</li> <li>41. FLADIS (Research on the Dispersion of Two-Phase Flashing Releases)</li> <li>42. Kincaid</li> <li>43. Bull Run</li> <li>44. Indianapolis</li> <li>45. Clifty Creek</li> <li>46. Tracy</li> <li>47. Martins Creek</li> <li>48. Westvaco</li> <li>49. SARMAP (San Joaquin Valley Air Quality Study, Regional Meteorological and Air Pollution)</li> <li>50. LMOS (Lake Michigan Ozone Study)</li> <li>51. OTAG (Ozone Transport Assessment Project)</li> </ol> |
|---|---|

\*Need to be requested from DoD

[www.admlc.com/datasets](http://www.admlc.com/datasets)



### Datasets

## Atmospheric Dispersion Datasets

Atmospheric dispersion datasets provide significant value in both the development and the validation & verification of atmospheric dispersion models. Furthermore, such datasets can be applied in sensitivity studies. This page of the website details summaries of, and descriptions how to access, publicly available atmospheric dispersion datasets. Access is either via a direct hyperlink to the dataset, by contacting the owner(s) of the data or by contacting the ADMLC Secretariat via [admlc@phe.gov.uk](mailto:admlc@phe.gov.uk). If you know of further datasets which could usefully be referenced on this page please contact the ADMLC Secretariat. Please note that ADMLC does not take responsibility for the quality of the data referenced here; it is the responsibility of the data user to determine the "quality" and applicability of the data.

### Modellers' Data Archive (MDA)

Fifty one different atmospheric transport and dispersion datasets are included in the Modellers' Data Archive (MDA) developed by Joseph Chang and Steven Hanna. These datasets can be obtained by contacting Joe ([jchang@rand.org](mailto:jchang@rand.org)) or Steve ([stevenrogershanna@gmail.com](mailto:stevenrogershanna@gmail.com)). An overview of the MDA is detailed in a presentation given by Joe Chang at the GMU Conference in 2016:

- <https://www.ofcm.gov/meetings/atd/gmu2016/pdf/10%20Chang.pdf>

### Search

### Meetings and Events

Meeting Dates:  
Next meeting: tba

Future meeting(s): tba

Seminar: –

Webinar: tba

<https://www.icams-portal.gov/meetings/atd/gmu2016/pdf/10%20Chang.pdf>



# Knowledge gaps exercise

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Collaborative exercise run in 2020 to identify topics for further research in Jack Rabbit III

Staged approach:

## 1. Pose open questions to gather information

- What is the issue?
- Why are we interested?
- What testing is needed?
- Example: Dry deposition
  - Some models predict it could have a significant effect on the hazard range
  - Lack of experimental data for dry deposition rates
  - Tests would involve measurements with different soil/vegetation samples downwind from large realistic release



# Knowledge Gaps Exercise

---

## 2. Group common issues identified in the responses into topics and sub-topics

- Five topic headings:
  - Source terms
  - Dispersion
  - Physicochemical effects
  - Mitigation
  - Outcomes

## 3. Contributors vote on their top three sub-topics

- For example, sub-topics in dispersion:
  - Obstacle effects
  - Terrain effects
  - Stable atmospheres
  - Internal boundary layers
  - Low wind speeds
  - Transition from dense to passive
  - Persistence in wakes/hollows
  - Detailed turbulence
- Contributors also asked which topics should not be studied



# Knowledge Gaps Exercise

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- 4. Collate responses from all contributors**
  - Votes summed to find highest-priority research topics
  - Specific research questions identified within the top five highest-priority sub-topics
  - Findings circulated for feedback from the contributors prior to finalising these slides

Findings presented at 24th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, 8-10 December 2020

<http://camp.cos.gmu.edu/>



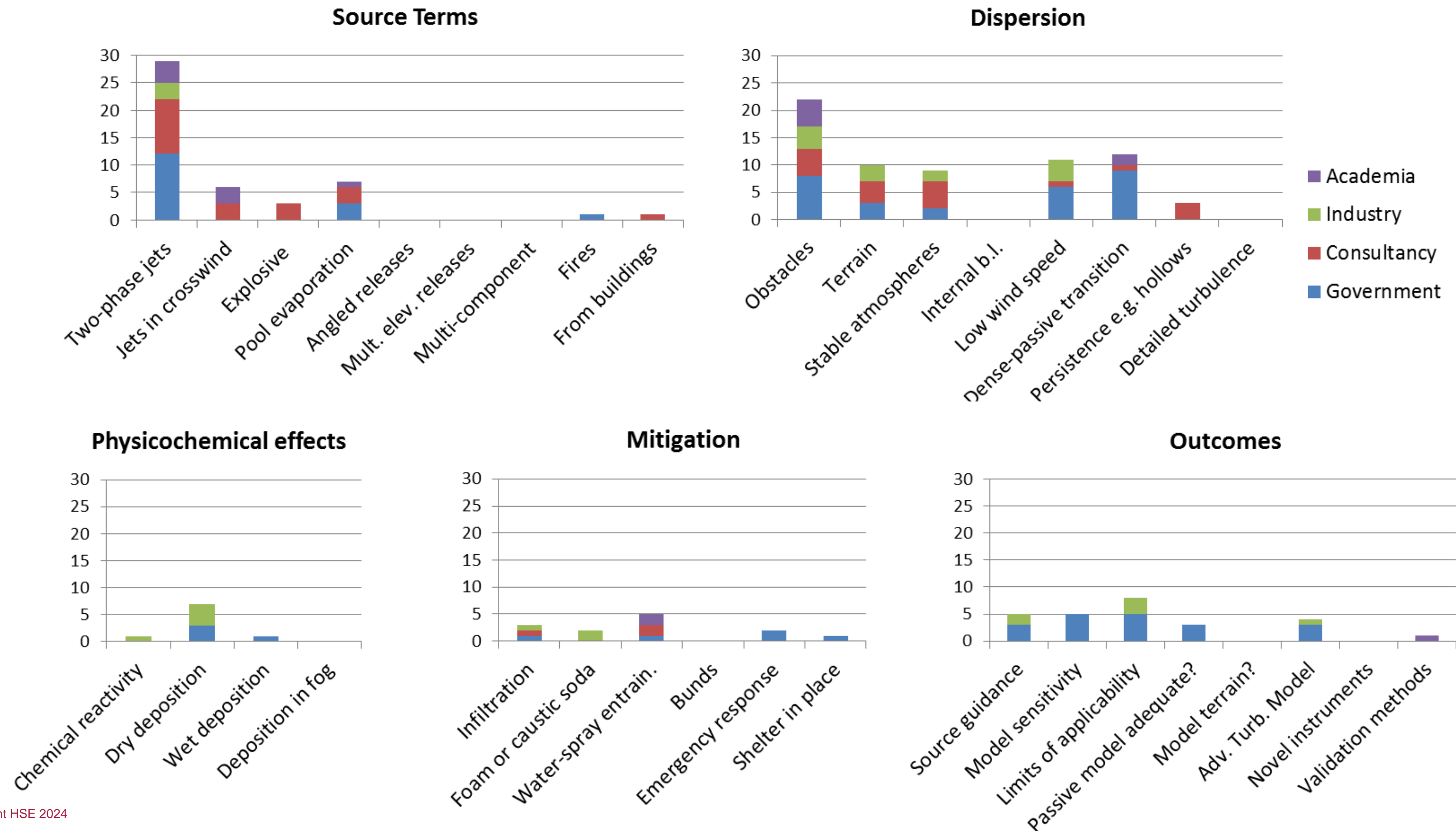
# Contributors

---

1. Maxime Nibart and Jacques Moussafir, **ARIA Technologies**, France
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19. Claire Witham and Susan Leadbetter, **Met Office**, UK
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22. Chris Dixon, **Shell**, UK
23. Stephen Puttick, **Syngenta**, UK
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25. Delphine Laboureur and Sophia Buckingham, von Karman Institute for Fluid Dynamics (**VKI**), Belgium

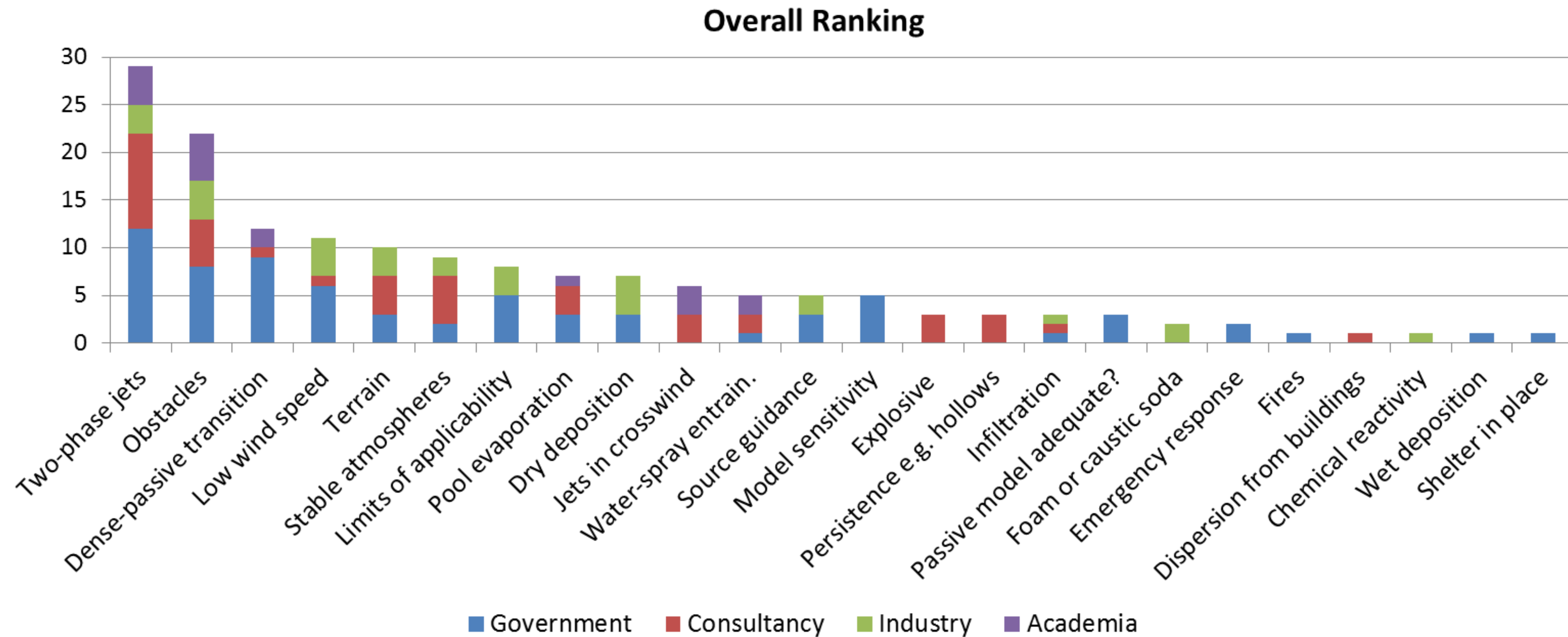


# Knowledge gaps: Results from votes



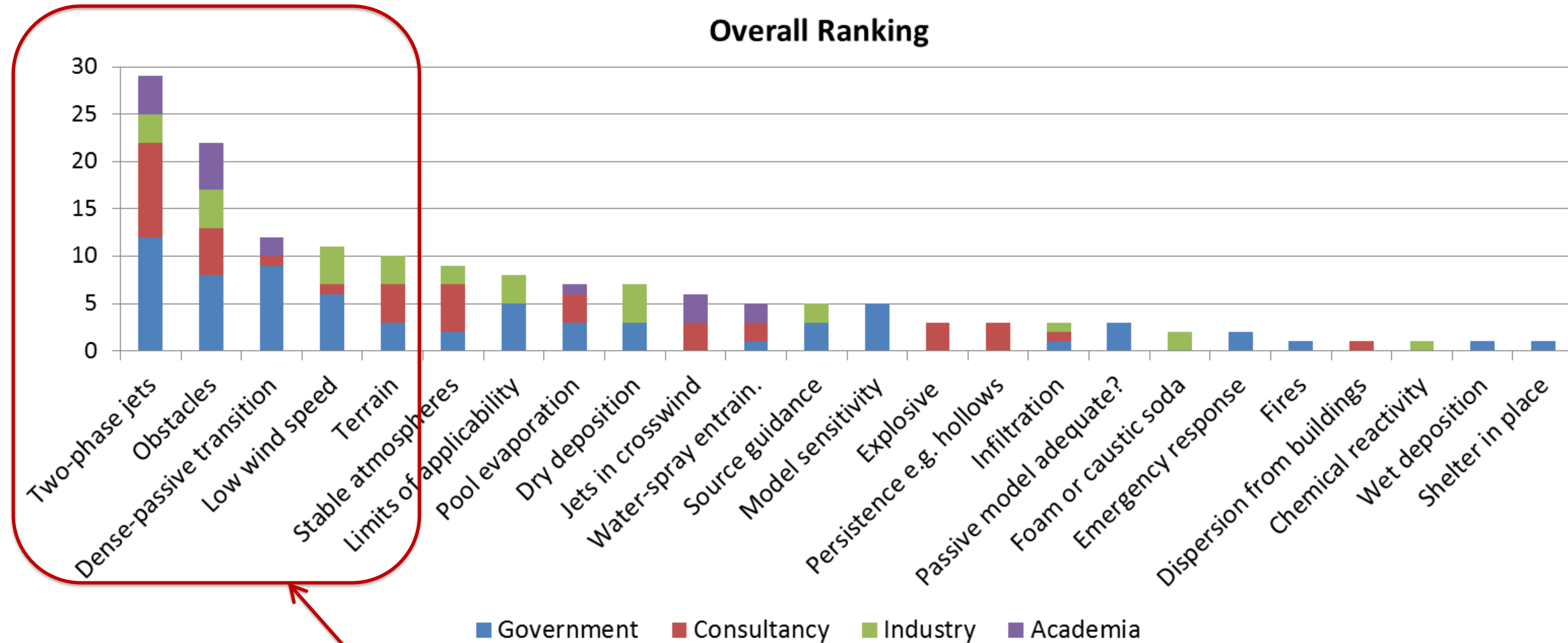


# Knowledge gaps: Results from votes





# Knowledge gaps: Results from votes



Next slides focus on top five sub-topics



# 1. Two-phase jets

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- Critical issue studied in several previous projects (see later review)
- Lack of data for partitioning between airborne aerosol and liquid pool (i.e. rainout fraction)
- Validity of rainout approaches in operational models is uncertain
- Rainout fraction can have significant influence on dispersion, particularly in the near field
- Rainout is scale-specific: depends on geometry and release size
- Useful to consider range of conditions: hole sizes, release orientations, impinging, short releases (e.g. catastrophic vessel failure), long duration releases (e.g. pipeline)
- Uncertainty in post-expansion source conditions: jet velocity and liquid fraction (metastable or homogeneous equilibrium) – could be studied in laboratory-scale tests?
- Uncertainty in behaviour inside vessel (champagne effect)



## 2. Obstacles

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- Limited field-scale data available for dense-gas dispersion with realistic obstacles
- At what size do obstacles become important such that they need to be taken account of in modelling?
- Are dense gas dispersion models for flat and rough terrain still applicable to built-up environments?
- Which is better: a building-resolved passive model or a dense gas model with surface roughness?
- How much do isolated or small obstacles affect dispersion?
- What is the impact of obstacles on persistence of the cloud?
- How effective are vapour barriers for mitigation?
- Do wakes from isolated tall buildings in city environments have a significant affect? Is it important to model them?



## 3. Transition from dense-gas to passive dispersion

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- When is it necessary to use a dense-gas model instead of a passive model?
  - Is the current rule of thumb that says a dense-gas model should be used for releases of 1 ton or more accurate?
- Can testing determine if there is a threshold release size when a passive model is adequate?
- How rapid is the mixing between the dense cloud and the atmosphere that produces a passive cloud?
- Does near-field dense gas behaviour matter far downwind?
- How does the transition from dense to passive affect turbulence levels and toxic dose (non-linear toxic response to concentration)?
- What are the implications for infiltration into buildings, e.g. draining of dense clouds into basements?



## 4. Dispersion in low/zero wind speeds

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- Lack of experimental data for large dense-gas releases in low/zero wind speeds
  - But there are examples of several severe incidents involving flammable dense-gas releases in low/zero wind, e.g. Buncefield and San Juan fuel storage depots
- How do obstacles and terrain influence the dispersion behaviour when the wind speed approaches zero?
- What are the implications of low/zero wind speeds for emergency response?
  - ERG provides protective action distance in downwind direction
  - ERG for ammonia has three wind speeds (low, moderate, high) for (<10 km/h, 10-20 km/h, >20 km/h)
  - What is the advice for very low or zero wind? Which direction is downwind? Are the ERG distances still valid?



## 5. Terrain effects

---

- Lack of experimental data for large dense-gas releases with terrain
  - Indications from incidents that even moderate slopes could have significant effect in low/zero wind
- At what scale does terrain become important for dispersion?
- What is the combined effect of the wind, the release direction and terrain on dense-gas releases?
  - Useful to have range of tests: e.g. releases upslope, downslope and cross-winds for a range of release sizes and slopes
  - Also elevated releases, e.g. for rooftop-mounted ammonia refrigeration tanks



# Knowledge gaps



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DOI: 10.1002/prs.12289

PROCESS SAFETY  
PROGRESS

## ORIGINAL ARTICLE

### Gaps in toxic industrial chemical model systems: Improvements and changes over past 10 years

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#### Funding information

Defense Threat Reduction Agency; Department of Homeland Security, Grant/Award Number: N/A; Health and Safety Executive

#### Abstract

To assess the hazards of the releases of toxic industrial chemicals (TICs) to the atmosphere, comprehensive model systems are often used, which begin with the scenario definition and end with an estimate of health risk. In 2008 and 2010, the US Department of Homeland Security and Defense Threat Reduction Agency sponsored reports that identified knowledge gaps in TIC modeling. The current paper discusses which of the knowledge gaps were satisfactorily resolved in the past 10 years by new theoretical and experimental research, such as the 2010 and 2015–2016 Jack Rabbit field experiments. For example, the linked source emissions and transport and dispersion (T&D) models have been shown, in comparisons with Jack Rabbit II observations, to not have large mean biases. Consequently, the T&D models are less likely to be the cause of model system overpredictions of casualties observed after large TIC accidental releases, such as the Festus, Macdona, and Graniteville chlorine railcar incidents. It may be that the deposition models and/or the health effects models still need improvement. In addition to comments on the knowledge gaps identified 10 years ago, a few new knowledge gaps are addressed, such as indoor T&D and deposition, and estimating the magnitude of the saturation deposition value for various substrates and chemicals.

#### KEYWORDS

anhydrous ammonia, chlorine, dense gas dispersion, hazards analysis, health risk, Jack Rabbit II field experiment, TIC

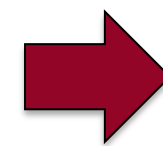
<http://dx.doi.org/10.1002/prs.12289>



# Ongoing HSE research activities

- Jack Rabbit III ammonia release experiments (2021-ongoing)
  - Led by US Departments of Homeland Security and Defense
  - Aims:
    - Conduct large-scale releases of ammonia, similar to Jack Rabbit II chlorine trials
    - Validate dispersion models
    - Improve preparedness of emergency responders
  - HSE co-chairs the Jack Rabbit III Modelling Working Group and has coordinated international dispersion model inter-comparison exercises

Images of previous series of Jack Rabbit II chlorine trials conducted in 2015-2016



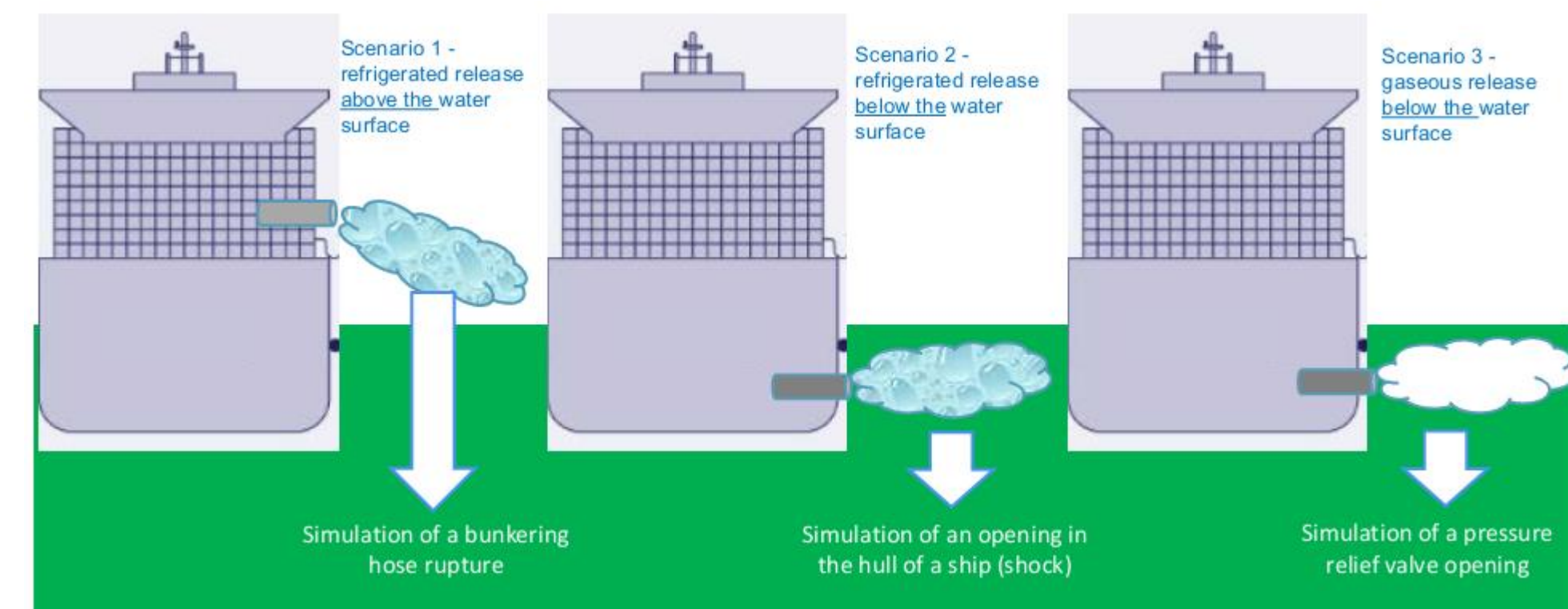
Images © DHS S&T CSAC and Utah Valley University  
<https://www.uvu.edu/es/jack-rabbit/>

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# Ongoing HSE research activities

- HSE is partner in the ARISE Joint Industry Project led by INERIS, Cedre and Yara
- Aims:
  - Conduct multi-tonne spills of ammonia at sea
  - Improve understanding of dispersion in water and air
  - Provide dataset for validation of models
  - Develop methodology for risk assessment for marine applications
- Tests planned for 2024-2025
- Contact: [Laurent.Ruhlmann@yara.com](mailto:Laurent.Ruhlmann@yara.com)







# Skylark CO<sub>2</sub> Dispersion Project

Simon Gant, Zoe Chaplin and Rory Hetherington (Health and Safety Executive, UK)  
Daniel Allason, Karen Warhurst, Ann Halford, Mike Harper, Jan Stene and Gabriele Ferrara (DNV)  
Tom Spicer (University of Arkansas, USA)  
Ed Sullivan (National Chemical Emergency Centre, UK)  
Justin Langridge and Matthew Hort (Met Office, UK)  
Steven Hanna (Hanna Consultants, USA)  
Joe Chang (RAND Corporation, USA)  
Gemma Tickle (GT Science and Software, UK)

**API Pipeline Conference, Salt Lake City, Utah, USA, 6-8 May 2024**



# Dense gas Terrain Modelling (DTM) project

- **Aim:** to develop a fast-running dense gas dispersion model that can simulate CO<sub>2</sub> pipeline releases in complex terrain, for use in risk assessment and emergency response



## Motivation

The development of Carbon Capture and Storage (CCS) infrastructure in the UK requires that new operational capabilities for dense-gas dispersion modelling be developed. For HSE, this capability is needed for the purpose of providing public safety advice on land-use planning to local authorities along the proposed routes of CO<sub>2</sub> pipelines and, potentially, around fixed installations, such as CO<sub>2</sub> capture plants. The Met Office delivers advice to emergency responders dealing with airborne hazards, such as potential future large-scale CO<sub>2</sub> accidents. Currently, the Met Office operate the [CHEMET service](#) using their NAME model for this purpose, but this model cannot simulate dense clouds, and an additional modelling capability would be needed to deliver such a service



## Deliverable

The model developers Riskaware, ESR Technology and GT Science & Software will deliver:

- Dispersion models that have been configured to simulate CO<sub>2</sub> releases from pipelines in complex terrain, with facilities to import UK terrain data.
- Documentation including a description of the underpinning physics, a software user guide and results from their model validation.

HSE, the Met Office and Dstl will deliver an evaluation of the models. This will consider the performance of the models (in terms of accuracy and speed) and the steps needed to integrate the models within their own systems.

Ultimately, the two models may prove to be complementary, with one model providing a quick solution for scoping studies and the other providing more granular detail of the CO<sub>2</sub> dispersion behaviour at higher computational cost. This will only become clear through the course of the project.

## Timescale

The DTM modelling project will run alongside the Skylark experimental project. It will start in Summer 2024 and run for three years until Summer 2027.

## Outline costs

ROM costs are currently estimated as £2-3 million, spread over three-year project duration.



# Thank you

## <Play Thorney Island videos>

<https://xnet.hsl.gov.uk/fileshare/public/3586/thorney-island-selection-v1-wmv.wmv>

<https://xnet.hsl.gov.uk/fileshare/public/3587/em00067-thorney-island-full-programme-edit-1982.mp4>

- 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
- Contact information: [simon.gant@hse.gov.uk](mailto:simon.gant@hse.gov.uk)



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# Extra material

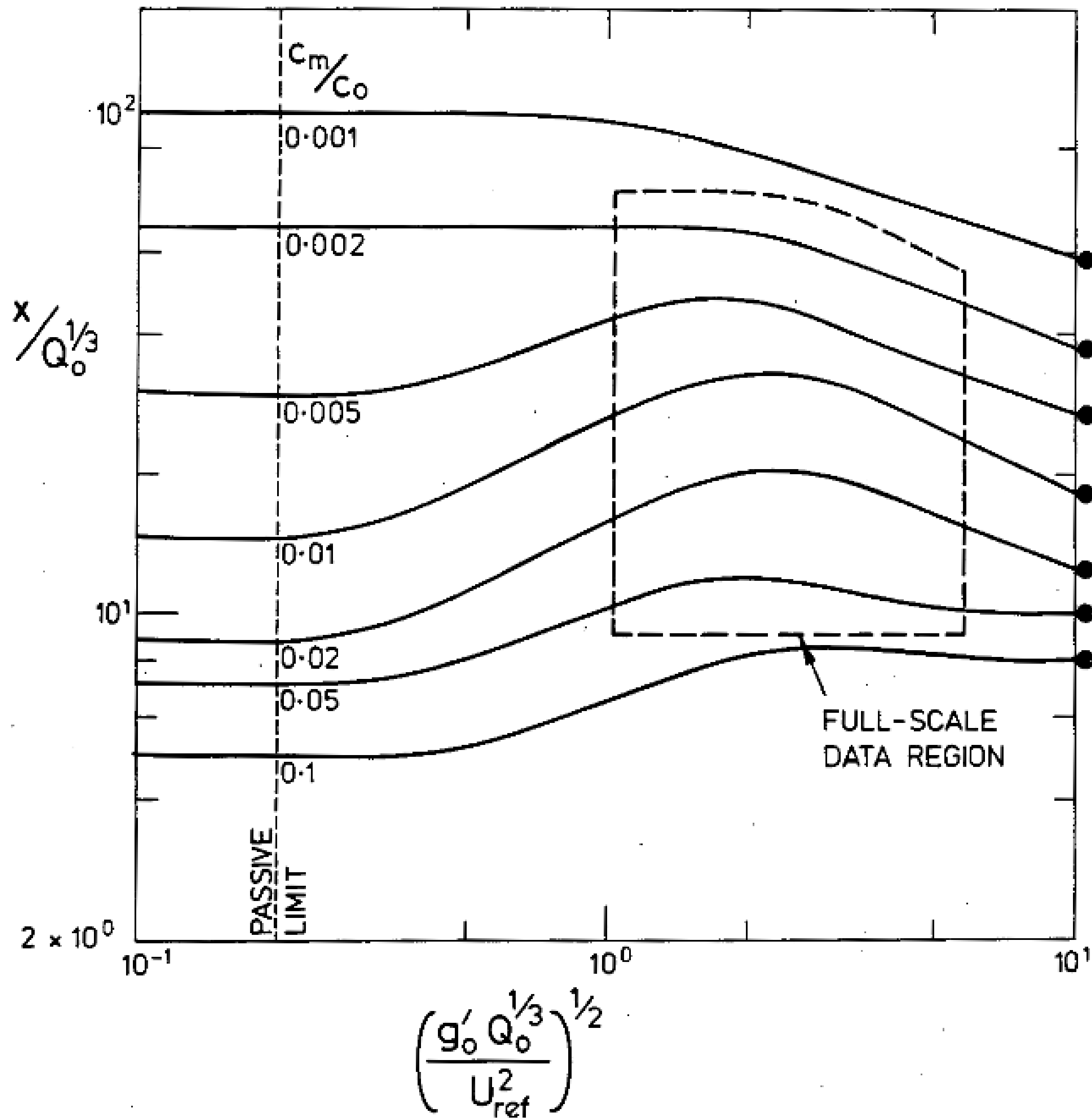


# Britter and McQuaid (1998)

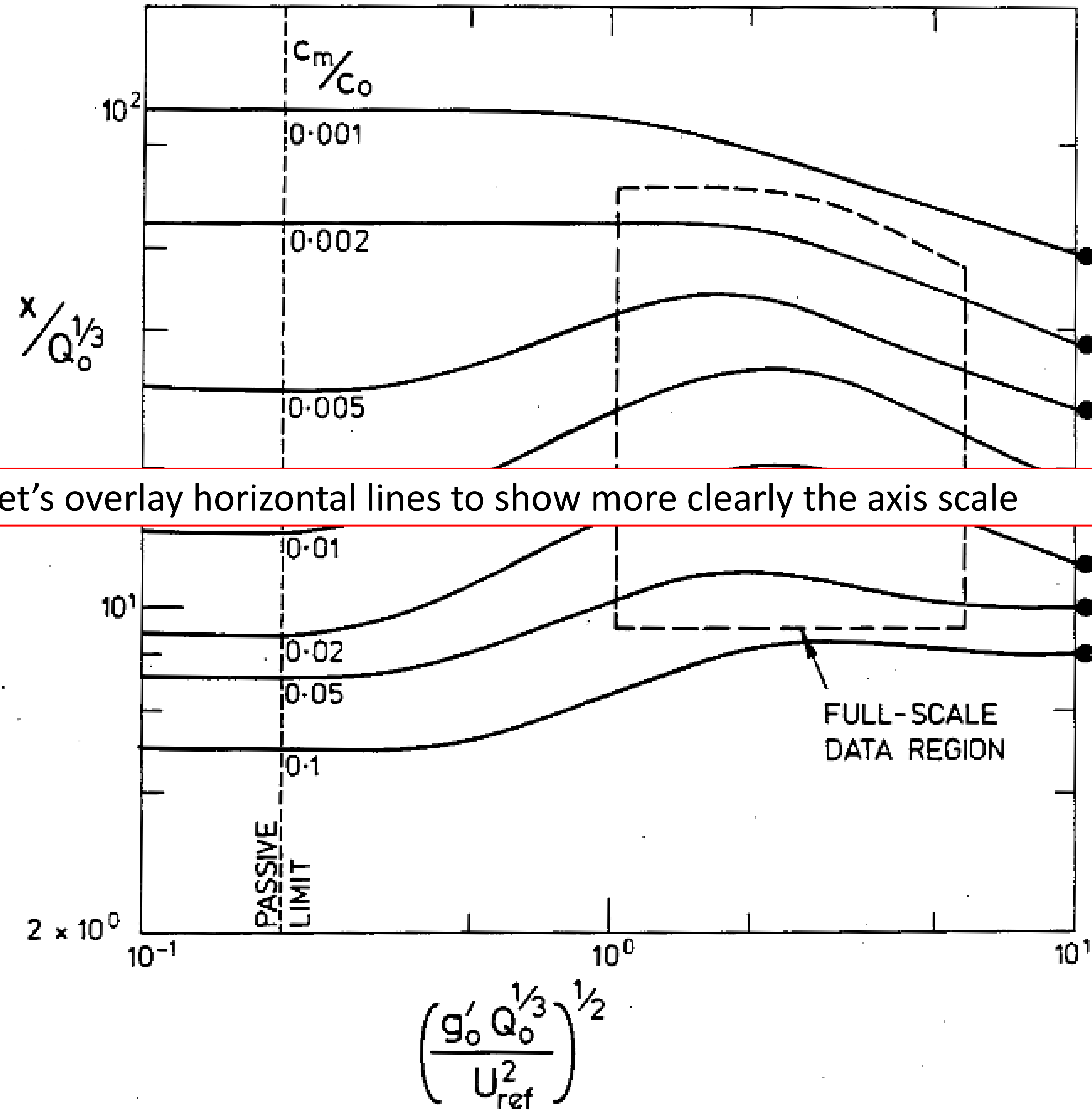
Investigating issues with the vertical  
axis scale Figure 11

Simon Gant, 29 May 2019



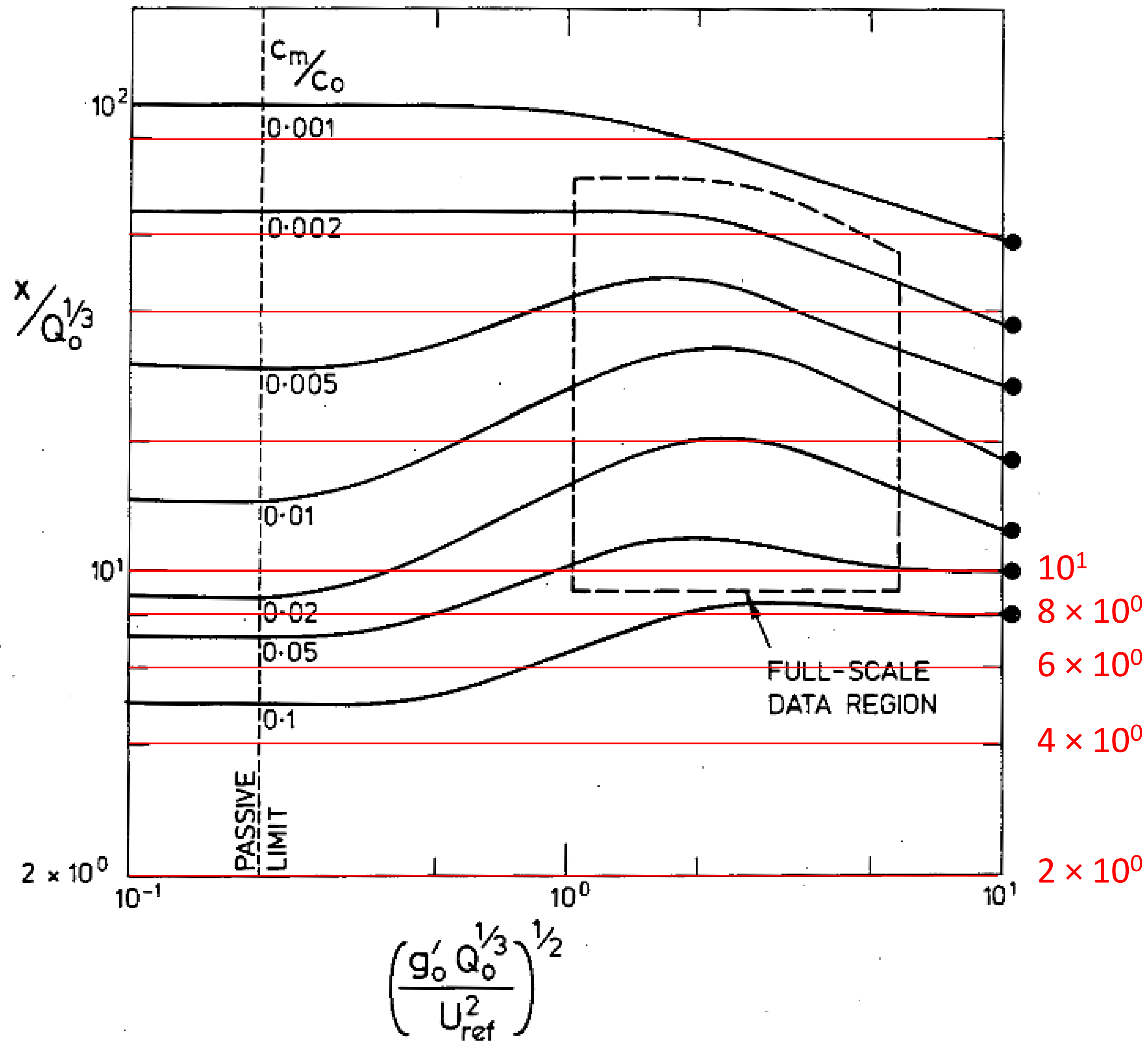




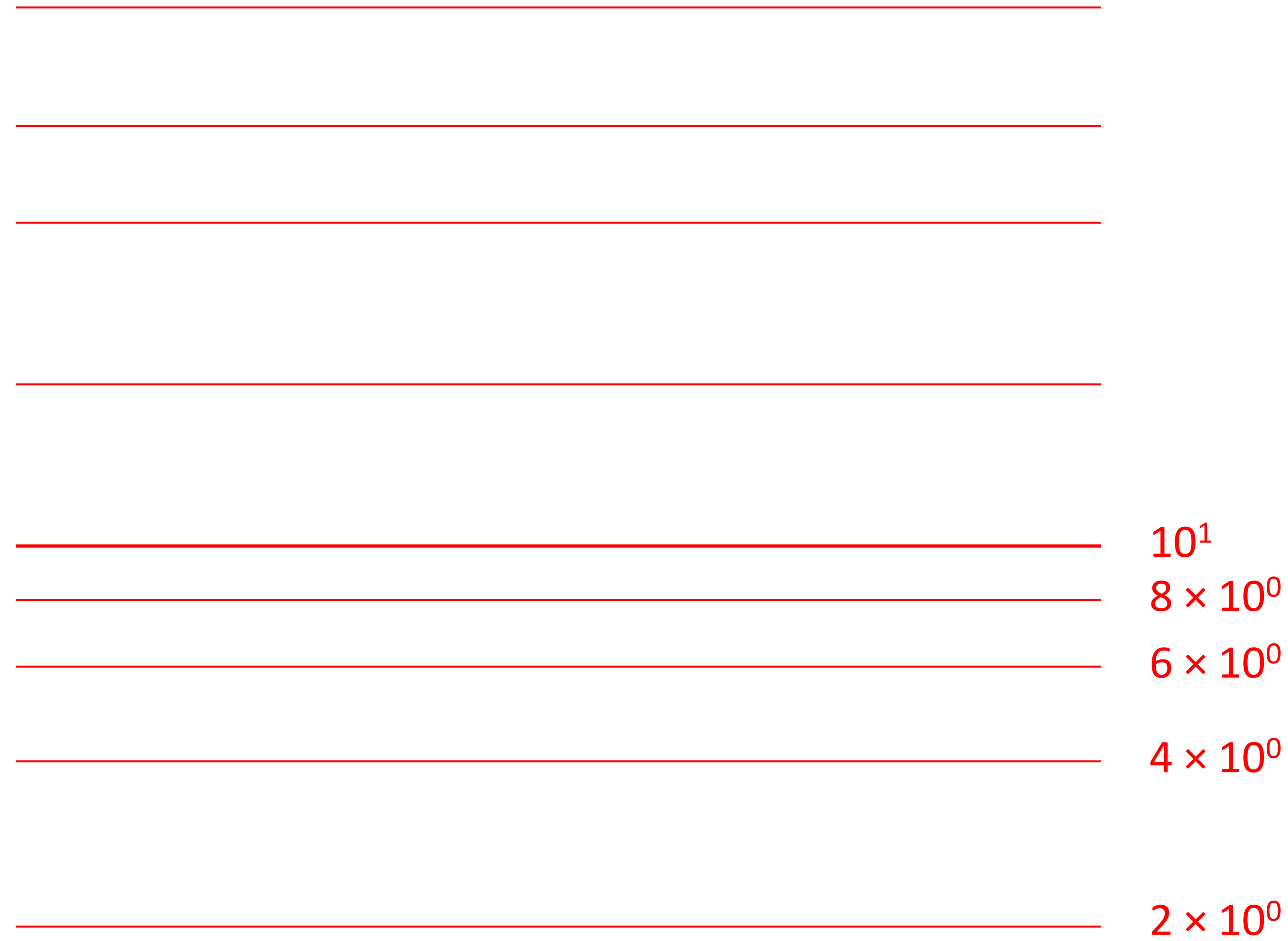


Let's overlay horizontal lines to show more clearly the axis scale



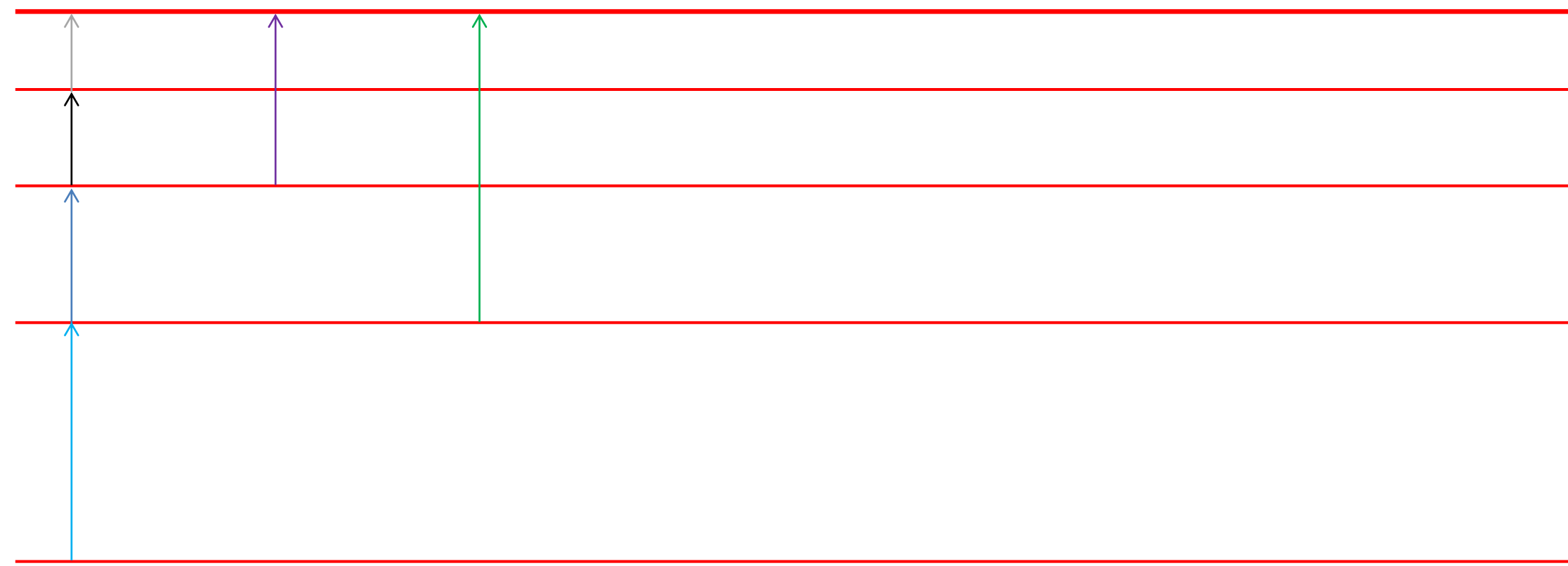
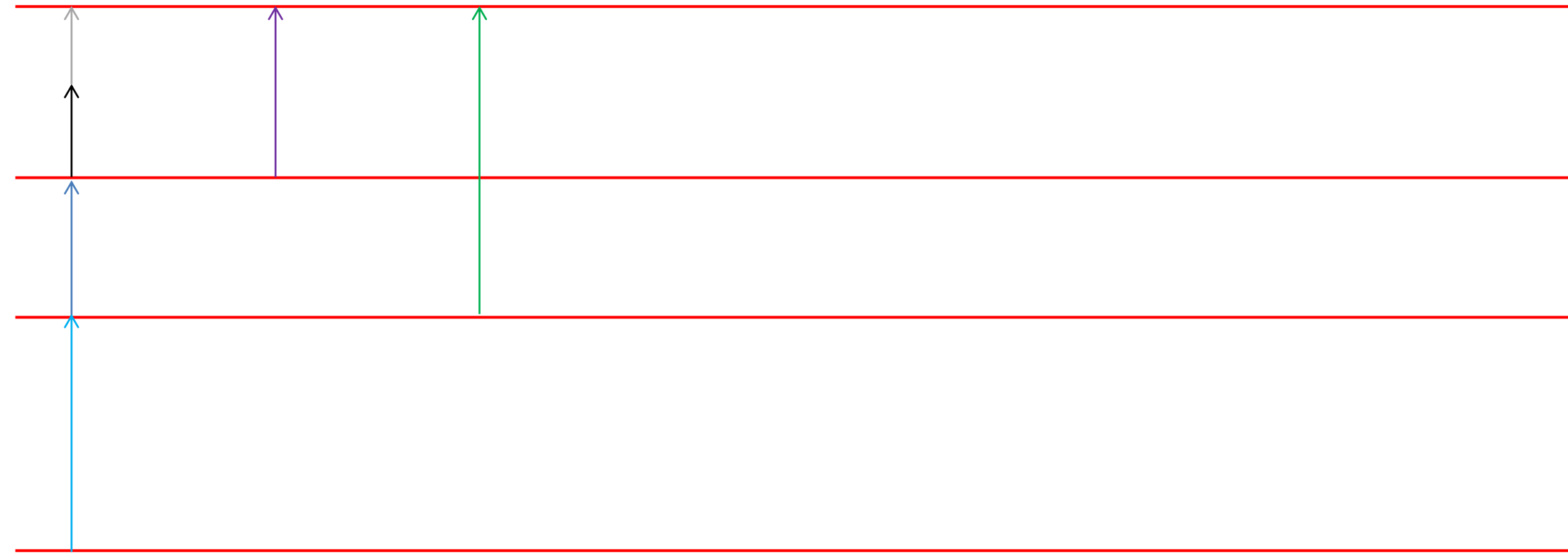






Let's measure distances between these lines and compare the lower range from  $2 \times 10^0$  to  $10^1$  with the upper range

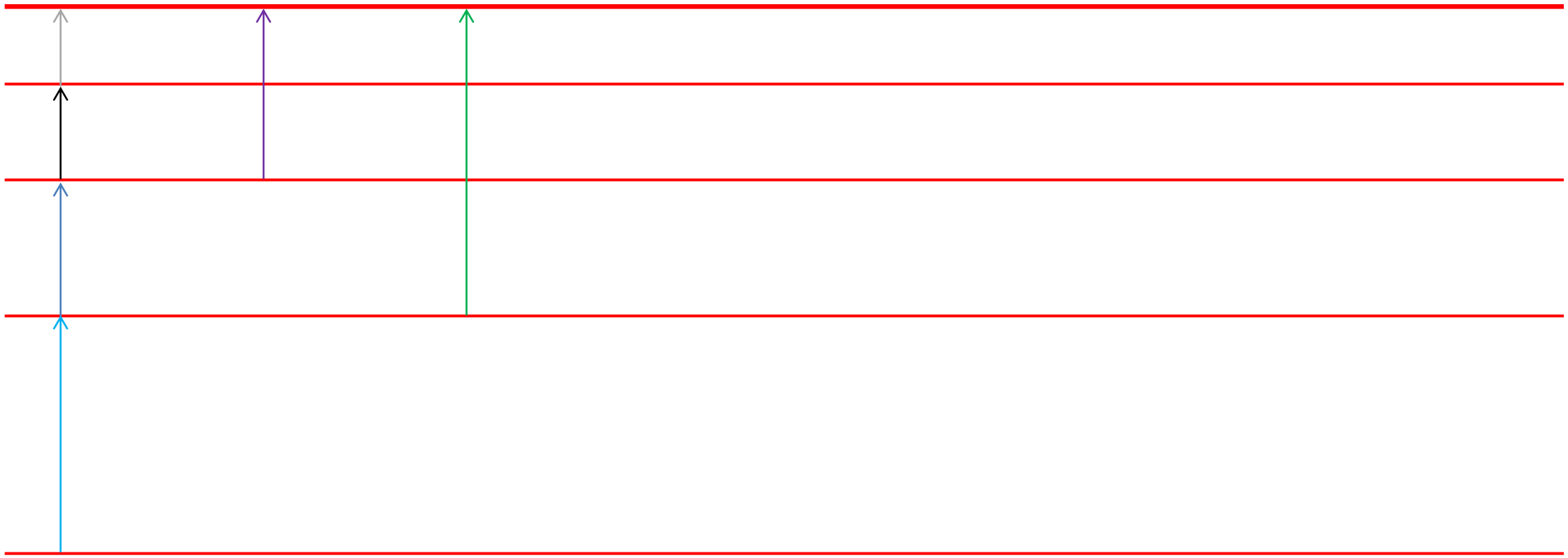
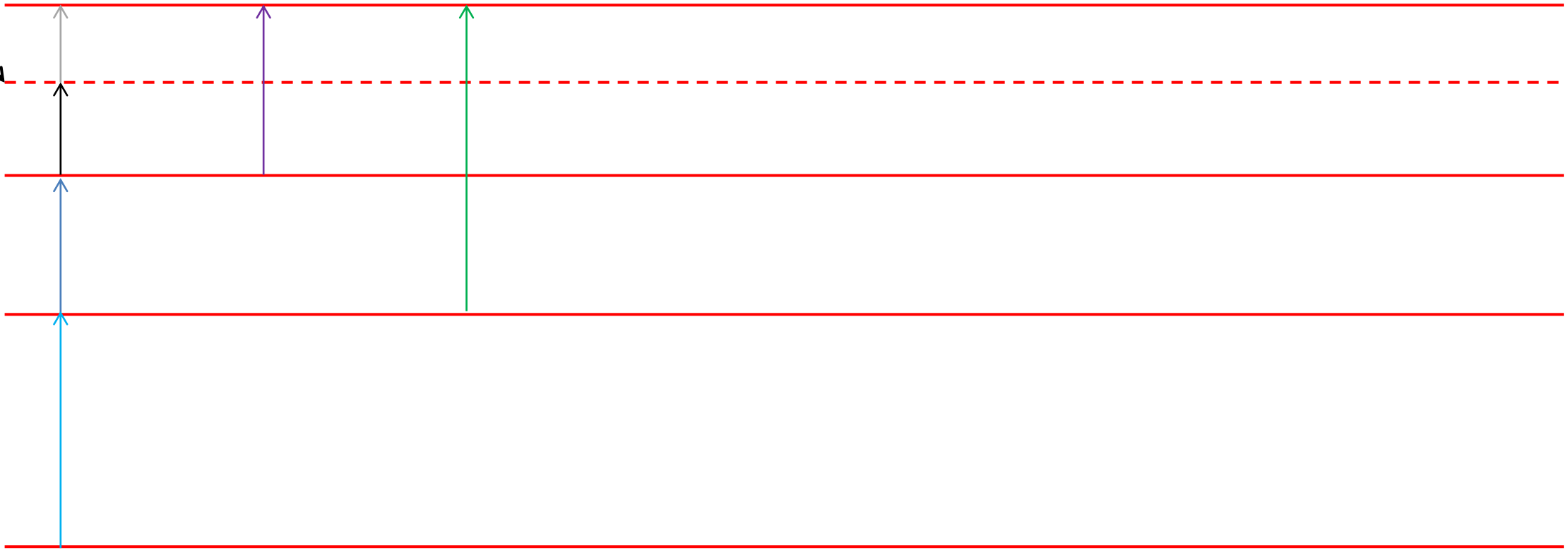
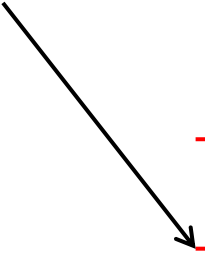




$10^1$   
 $8 \times 10^0$   
 $6 \times 10^0$   
 $4 \times 10^0$   
 $2 \times 10^0$



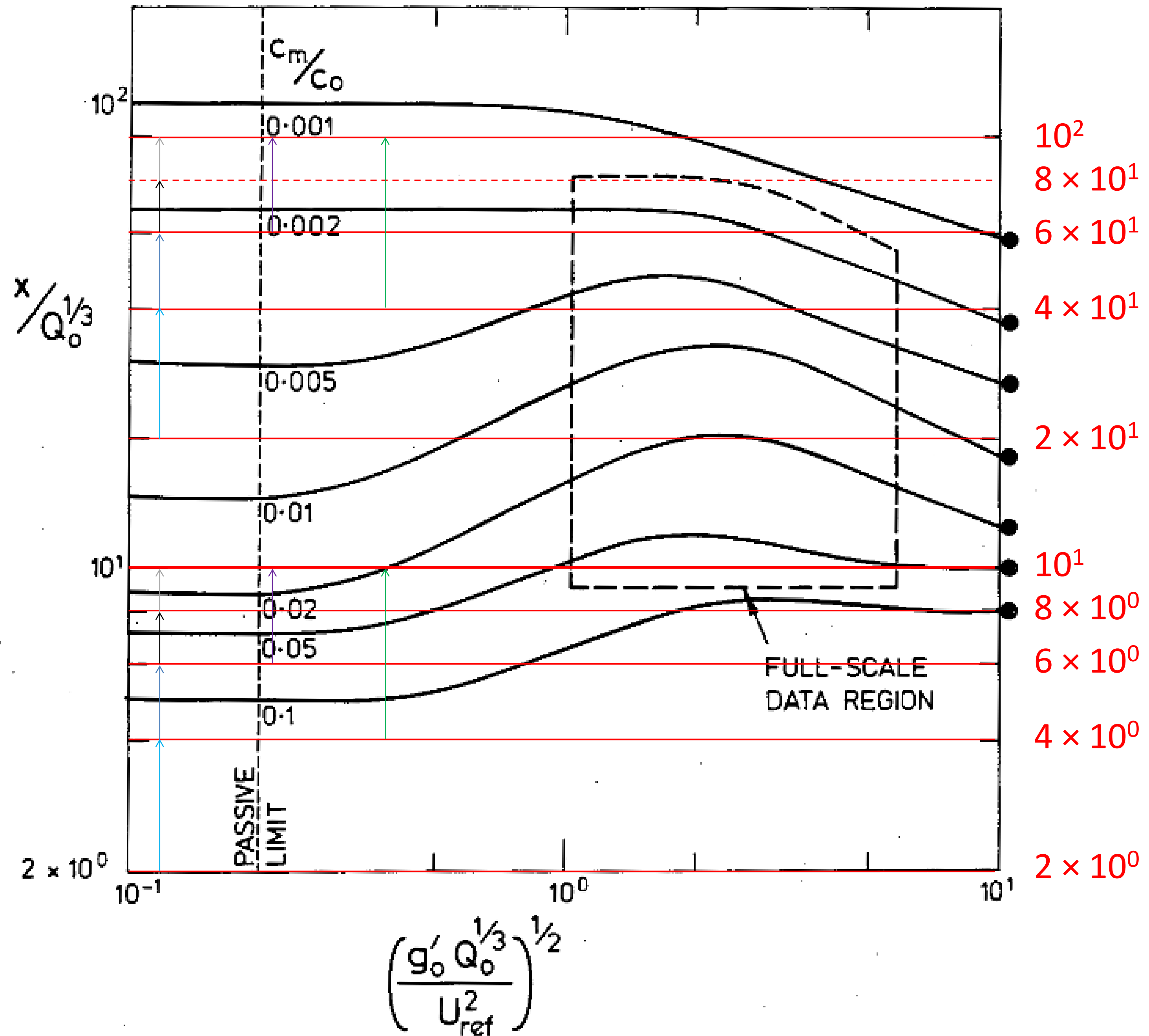
It looks like this dashed line is missing...



$10^1$   
 $8 \times 10^0$   
 $6 \times 10^0$   
 $4 \times 10^0$   
 $2 \times 10^0$

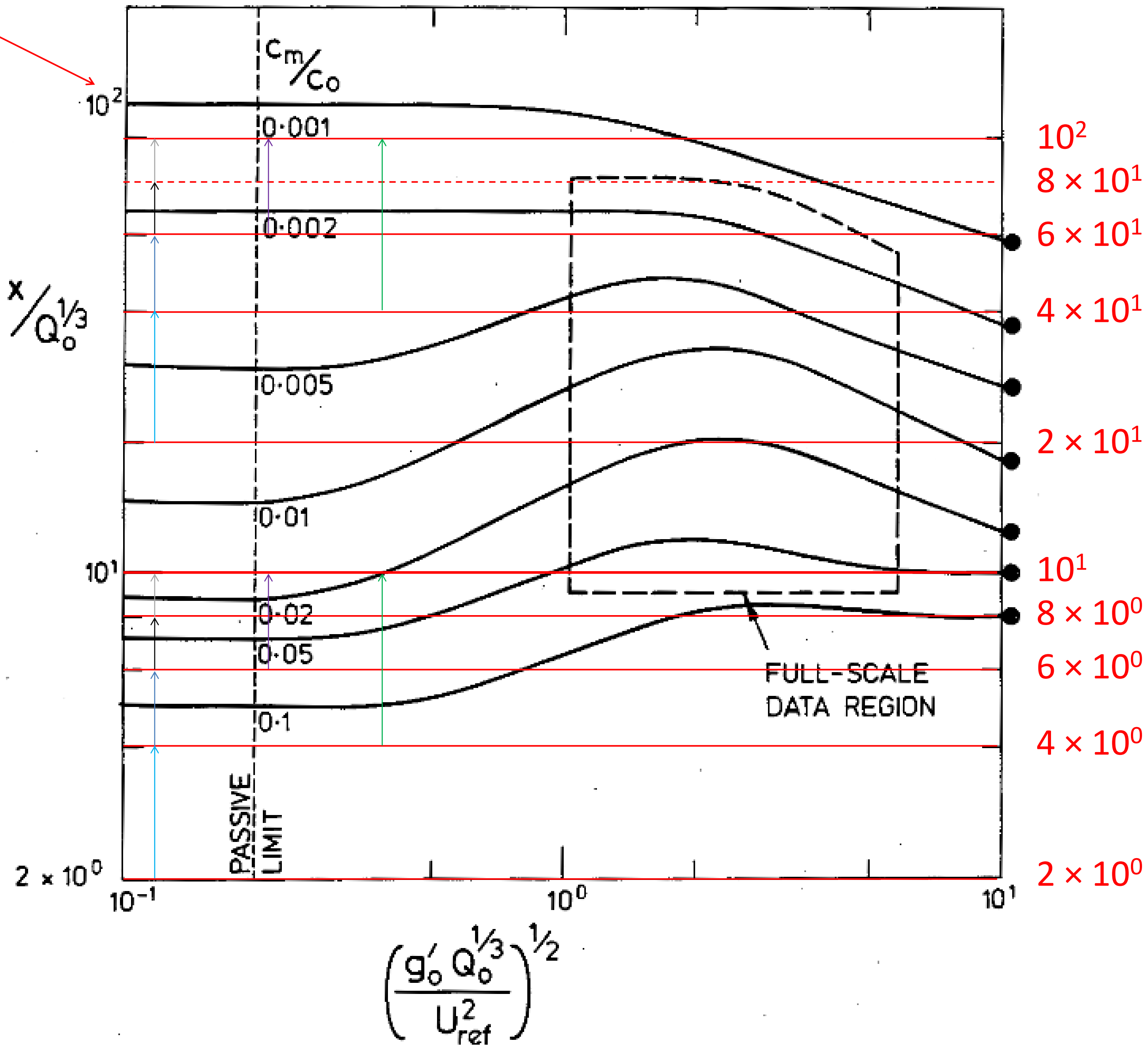
Let's superimpose that back on the Britter and McQuaid figure







This text "10<sup>2</sup>" should be moved down to the nearest tick mark below





Corrected version

"10<sup>2</sup>" moved

Missing tick added

