RESEARCH AND GUIDANCE FROM HSE

Phast modelling of the Desert Tortoise and FLADIS ammonia trials for the Jack Rabbit III model inter-comparison exercise

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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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- JRIII modelling exercise participants who used Phast
- Phast capabilities overview
- Modelling approach taken by different groups
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Phast modellers

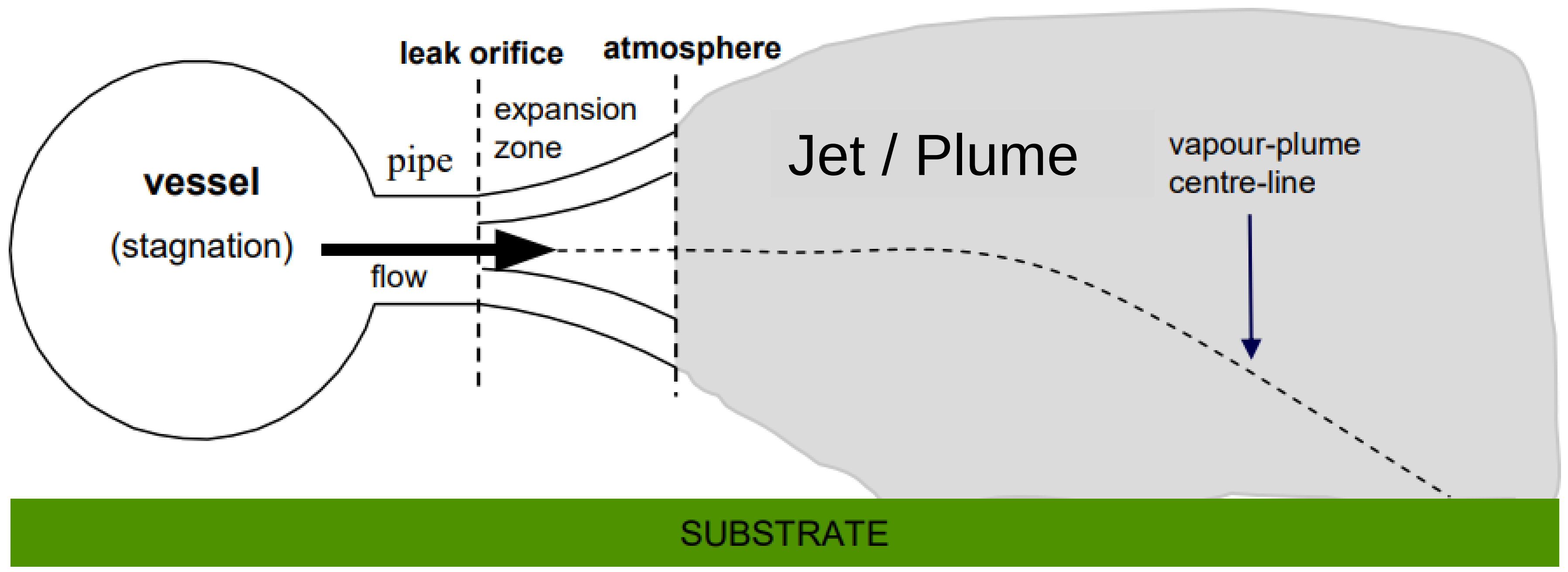
- Five groups used the DNV Phast software for the JRIII model inter-comparison exercise on Desert Tortoise and FLADIS
- Each group worked independently
- Meeting held to discuss modelling approach and results on 16 May 2022
- Follow-on emails and Teams discussions
- Equinor joined the exercise in June 2022

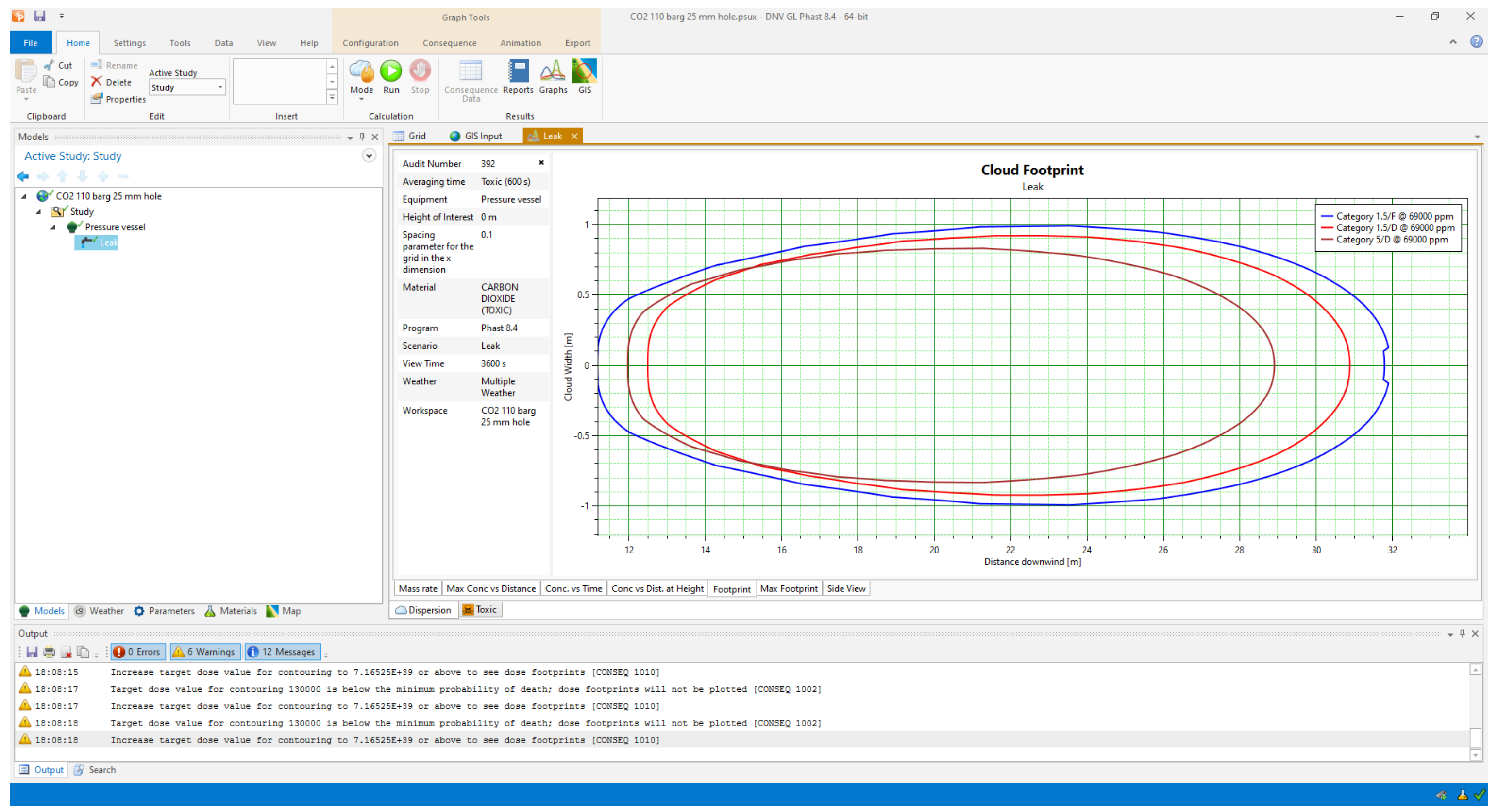
Group	Phast Version	Modellers
DGA, France	8.6	Laurent Verdier
DNV, UK	8.61	Frank Hart & Mike Harper
HSE, UK	8.4	Alison McGillivray
Syngenta, UK	8.61	Adeel Ibrahim & Stephen Puttick
Equinor, Norway	8.6	Sandra Nilsen

Version 8.61 is currently the latest release

Phast overview

- Phast is one of the most popular consequence models used in UK/Europe for assessing industrial major accident hazards at oil/gas/chemical facilities
- Software features:
  - Source models for releases from: vessels, short pipes and long pipelines, pool spread and evaporation
  - Unified Dispersion Model: two-phase jets, buoyant/heavy and passive dispersion, droplet rainout
  - Models for time-dependent releases: steady-state, finite-duration, instantaneous or time-varying
  - Assumes flat terrain with uniform surface and constant atmospheric conditions





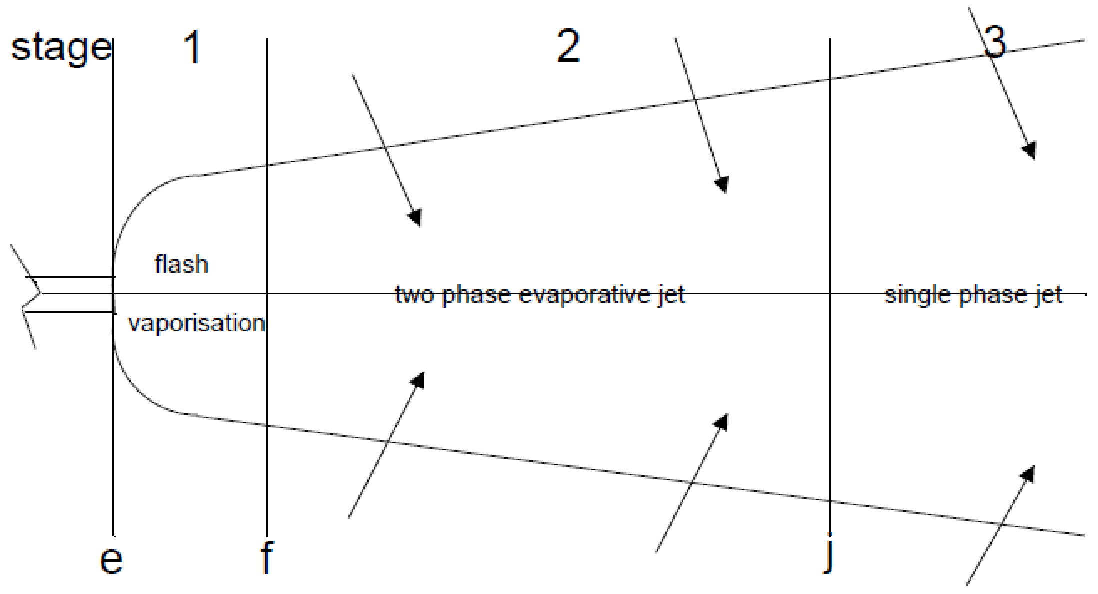
Model input conditions

- Modellers used conditions as specified by the JRIII exercise coordinators, but several different modelling approaches taken
  - Syngenta and Equinor were the only groups who took the same approach

Group	Post-expansion two-phase source from SMEDIS project?	User-defined source with corrected mass flow rate?	Manually adjusted orifice diameter to give correct mass flow rate	Release conditions at bubble point (ambient temperature)	Phast core averaging time matched specified averaging time?	Isenthalpic or "conservation of momentum" expansion model	Phast version
DGA	No	No	No[1]	Yes[2]	No	Isenthalpic	8.6
DNV	Yes	No	No	No	Yes	N/A	8.61
HSE	No	Yes	No	No	Yes	Isenthalpic	8.4
Syngenta	No	No	Yes	No	No	Isenthalpic	8.61
Equinor	No	No	Yes	No	No	Isenthalpic	8.6

[1] DGA modelled a fixed duration release based on the specified release duration and release rate, which meant that Phast itself determined the necessary orifice size

[2] DGA initially specified the source conditions using the exit pressure and temperature, but then changed this in the Phast interface to be the bubble point (saturation) conditions at the ambient temperature. However, this change led to some cases being modelled as a vapour release rather than a liquid release.



Model input conditions

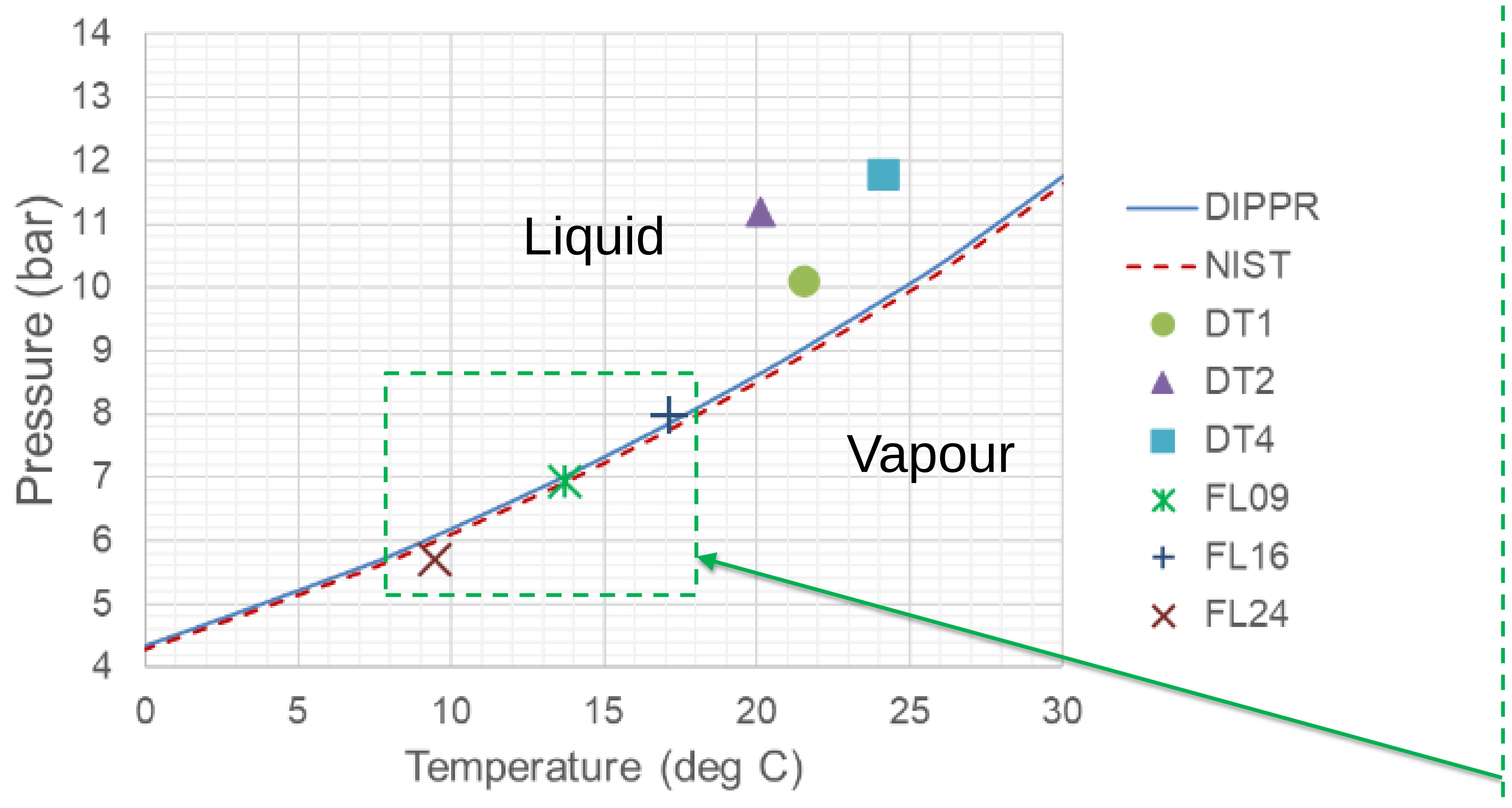
- What was the modelling issue with the exit pressure and temperature?

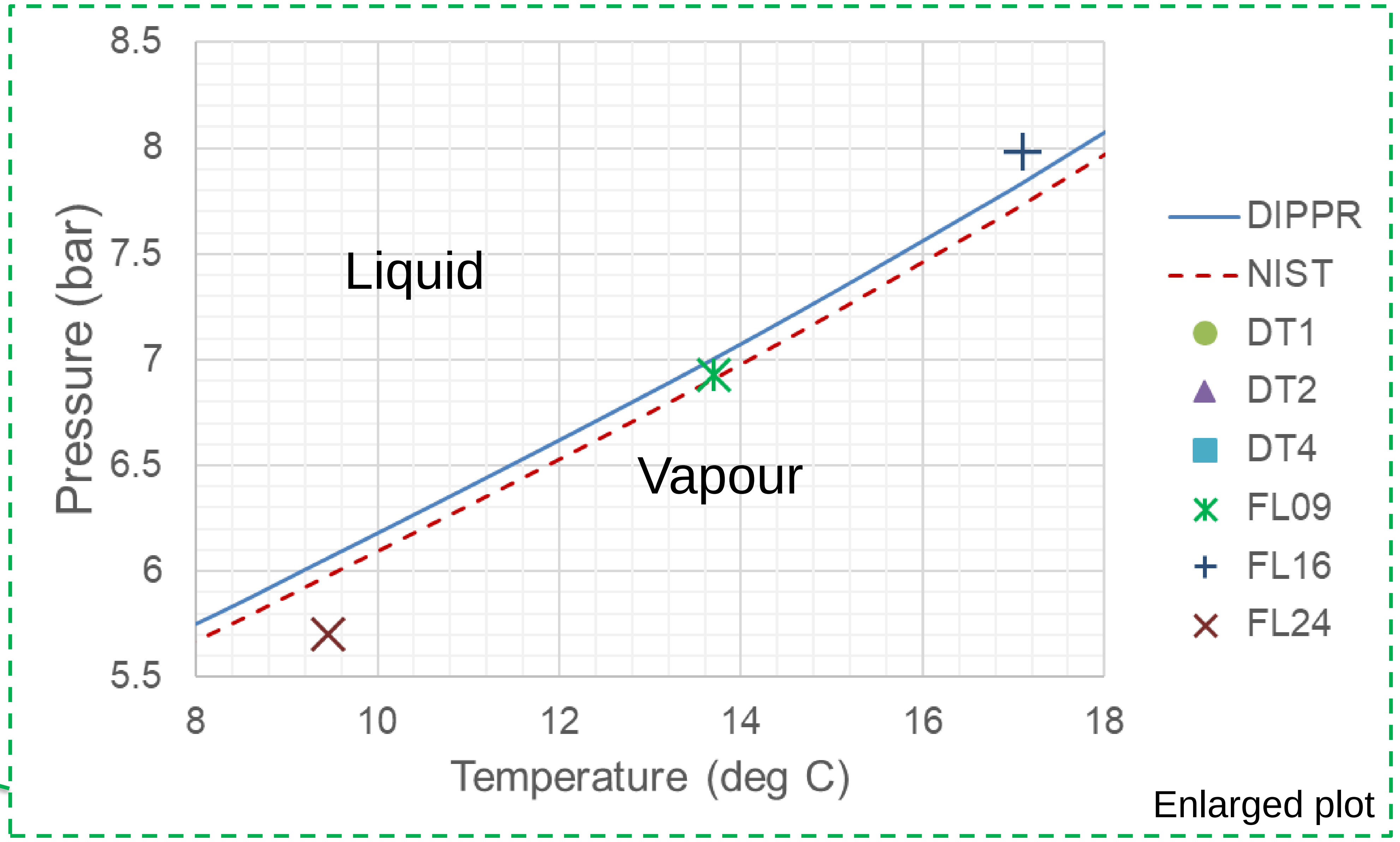
		DT1	DT2	DT4	FLADIS9	FLADIS16	FLADIS24
Orifice diameter	m	0.081	0.0945	0.0945	0.0063	0.004	0.0063
Release height	m	0.79	0.79	0.79	1.5	1.5	1.5
Exit temperature	°C	21.5	20.1	24.1	13.7	17.1	9.45
Exit pressure	bara	10.1	11.2	11.8	6.93	7.98	5.70
	barg	9.22	10.3	10.9	5.91	6.96	4.69
Release rate	kg/s	80.0	117	108	0.40	0.27	0.46
Release duration	s	126	255	381	900	1200[g]	600
Rainout mass fraction	%	5	5	5	0	0	0
Site average wind speed	m/s	7.42	5.76	4.51	6.1	4.4	4.9
at reference height	m	2	2	2	10	10	10
Friction velocity	m/s	0.442	0.339	0.286	0.44	0.41	0.405
Surface roughness	m	0.003	0.003	0.003	0.04	0.04	0.04
Monin-Obukhov length	m	92.7	94.7	45.2	348	138	-77
Pasquill stability class	-	D	D	D-E	D	D-E	C-D
Ambient temperature	°C	28.8	30.4	32.4	15.5	16.5	17.5
at reference height	m	0.82	0.82	0.82	1.5	1.5	1.5
Ambient pressure	bar	0.909	0.910	0.903	1.020	1.020	1.013
Relative humidity	%	13.2	17.5	21.3	86	62	53.6
Averaging time for mean values	s	80	160	300	600	600	400

Source: JRIII initial modeling exercise description v2.3.pdf

Model input conditions

- The specified exit pressure and temperature for FLADIS trials 9 and 24 were in the vapour phase according to the phase diagram used by Phast, so these were modelled as vapour releases by all groups except DNV
  - In reality, the Desert Tortoise and FLADIS exit conditions were approximately 100% liquid
  - Exit conditions were in the vapour phase probably as a result of either non-equilibrium conditions or the pressure and temperature being measured at slightly different locations in the experiments





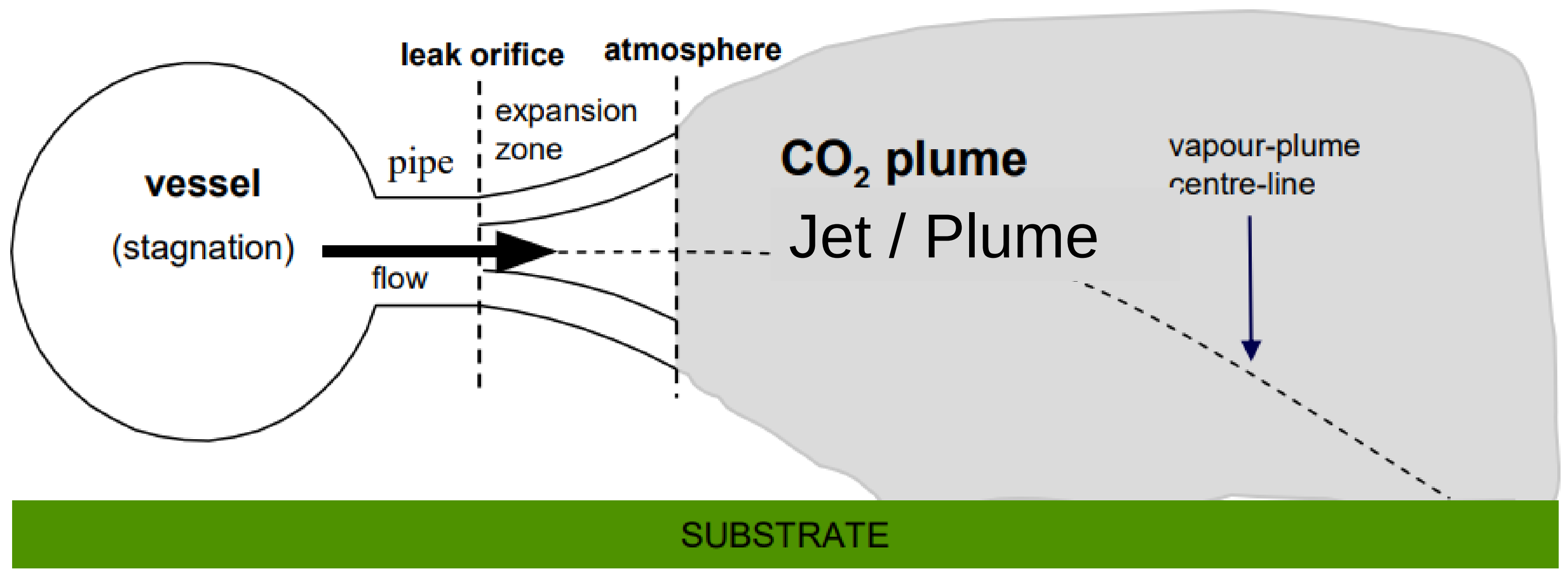
Phast uses DIPPR for the saturation conditions: https://chemicals.readthedocs.io/chemicals.dippr.html
Alternative correlation shown from NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=C7664417&Mask=4#Thermo-Phase

Post-expansion source conditions

High velocity from default isentropic expansion model

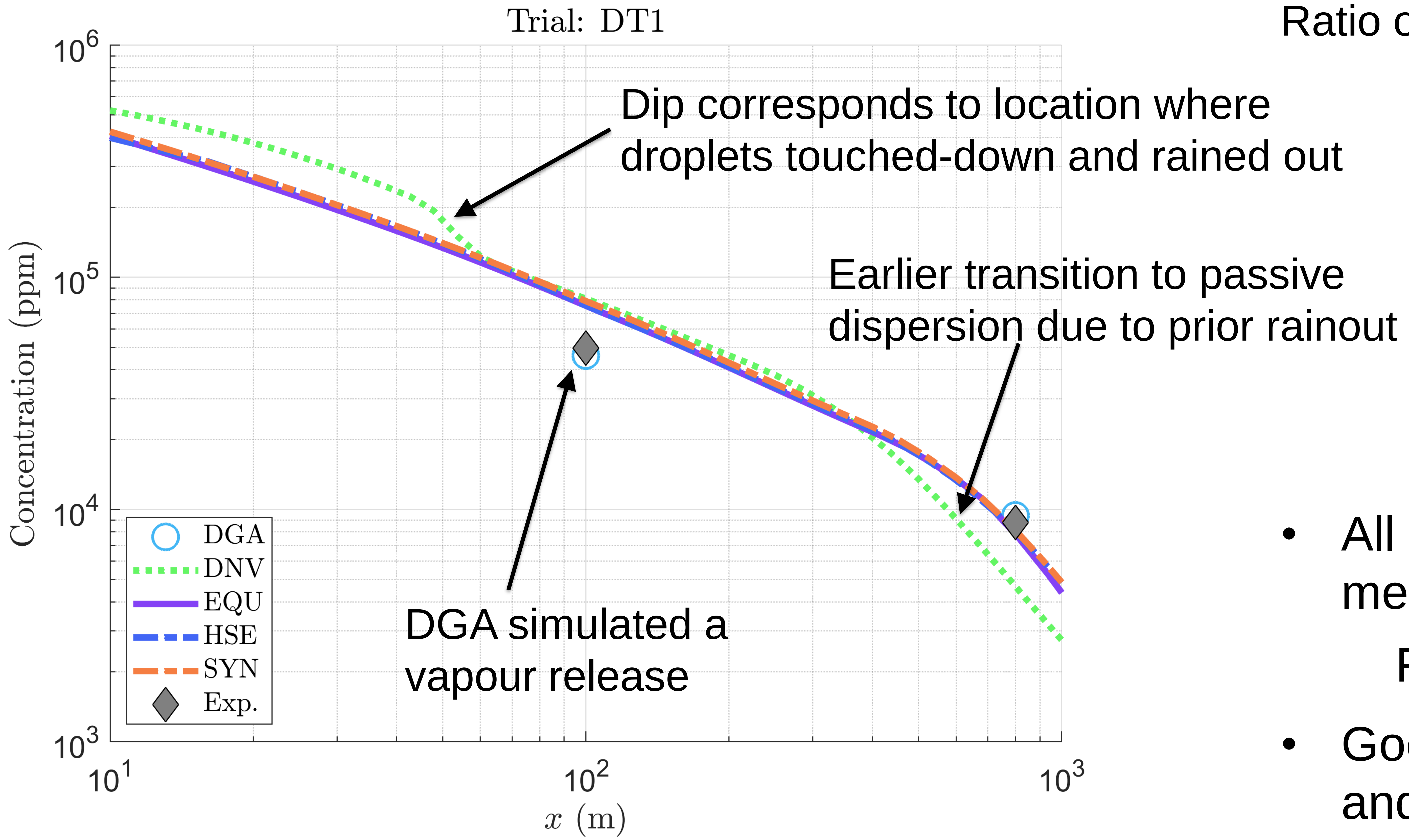
Lower velocity from SMEDIS source ("conservation of energy model" in Phast would also predict a similarly low velocity)

	Desert Tortoise DT1				FLADIS FL9			
	HSE	DNV	Syngenta	DGA	HSE	DNV	Syngenta	DGA
Final velocity (m/s)	246	90.3		663	617	65.2	617	624
Liquid fraction	0.825	0.82		0.09	0.082	0.84	0.08	0.09
Droplet diameter (µm)	83.7	107		0.94	0.91	144	0.9	0.9



High velocity, low liquid fraction and small droplets (from condensation) all indicate a vapour release was modelled by Phast in these four cases

Results: Desert Tortoise trial 1



Concentrations output from Phast at a height of 1 m above ground level (the height of the sensors in the experiments)

Ratio of predicted to measured arc-max concentrations

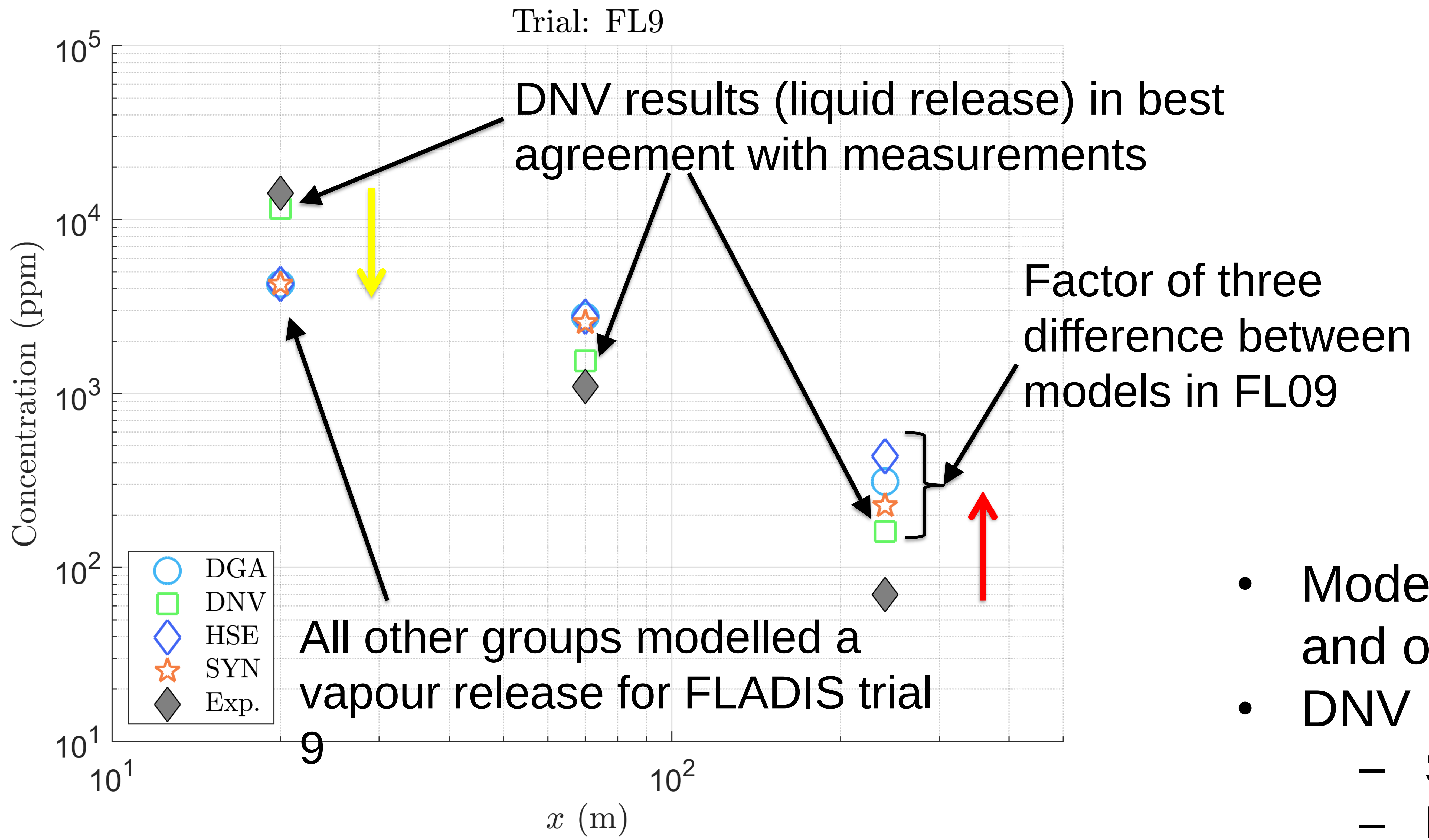
x (m)	C_p/C_m			
	DGA	DNV	HSE	SYN
100	0.93	1.63	1.53	1.60
800	1.07	0.53	0.91	0.92

- All predictions within a factor-of-two of the measurements

  FAC2 condition: $0.5 \leq \frac{C_p}{C_m} \leq 2$

- Good agreement between model predictions and measurements

Results: FLADIS trial 9



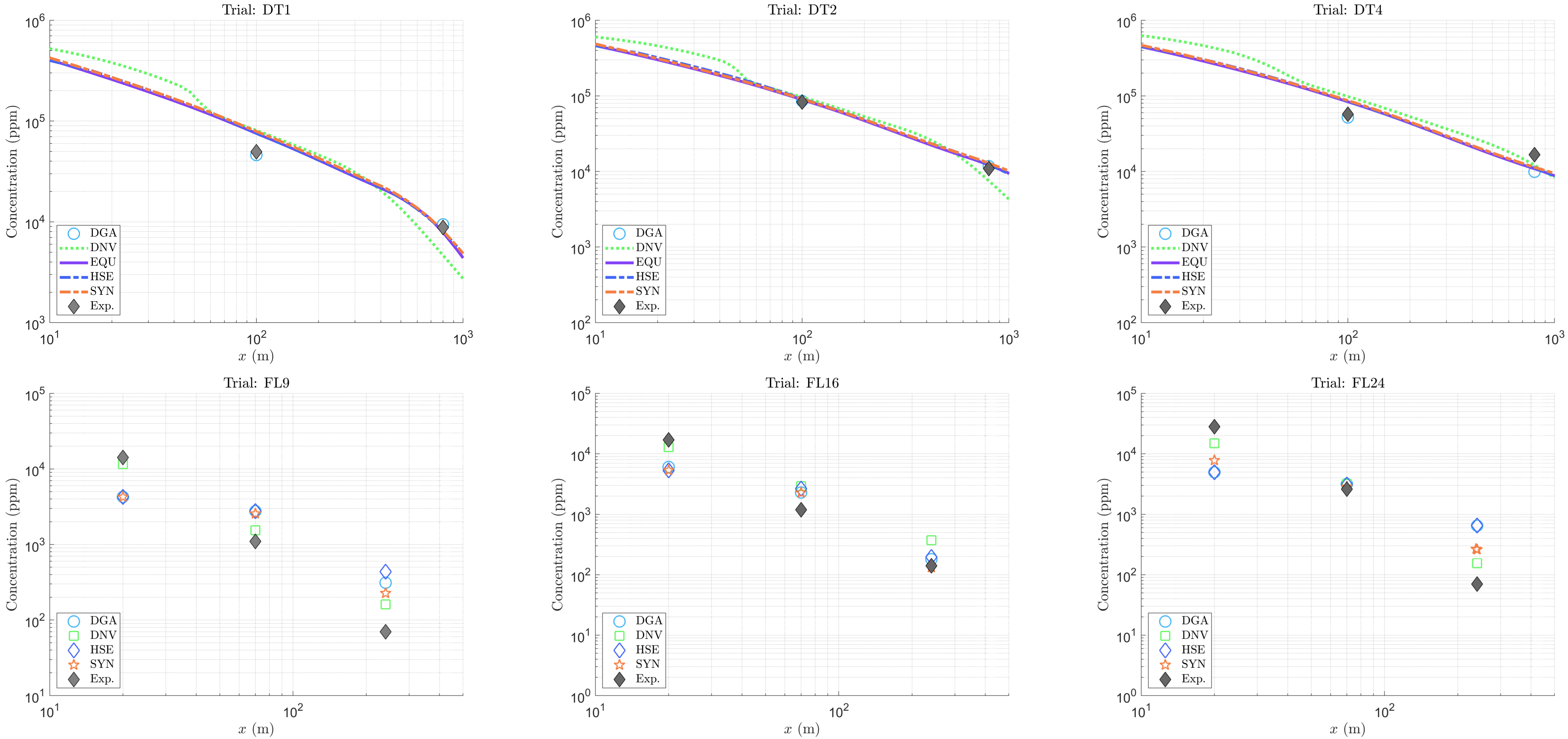
Ratio of predicted to measured arc-max concentrations

x (m)	C_p/C_m			
	DGA	DNV	HSE	SYN
20	0.30	0.82	0.30	0.30
70	2.51	1.40	2.51	2.32
238	4.44	2.30	6.24	3.24

- Models under-predicted measurements near orifice, and over-predicted measurements further downstream
- DNV model performs best
  - SMEDIS two-phase source for liquid release was used
  - More than half of DNV predictions within factor of two of measurements over all of the FLADIS trials

Concentrations output from Phast at same height as measurements, i.e., heights of 0.1 m, 0.5 m, 1.5 m at distances of 20 m, 70 m, and 238 m (or 240 m)

All Desert Tortoise and FLADIS Results



Recommended Phast modelling approach going forward

Based on discussions with Phast software developers at DNV, recommendations provided for how best to use Phast for pressure-liquefied releases:

1. Check the specified orifice exit pressures and temperatures on a phase diagram to confirm that the conditions input to Phast produce the expected phase of the ammonia released in the experiments (i.e., liquid or vapour). Also check the predicted liquid fraction in the Phast results.
2. Set the core averaging time to be the same as the specified toxic averaging time.
3. For cases with rainout, find the initial post-expansion ammonia droplet diameter by running a simulation using the default isentropic expansion model and the CCPS droplet size correlation
4. Re-run the same Phast case using the conservation of momentum atmospheric expansion model, which gives a more representative post-expansion source velocity
5. Produce a user-defined source from Step 4 and change the droplet size to that found from Step 3, and then run Phast. This approach will use the best estimate for the release velocity and droplet size.

Conclusions

- Five modelling groups (DGA, DNV, HSE, Syngenta and Equinor) produced results using Phast for the JRIII modelling exercise on Desert Tortoise and FLADIS
- Several different modelling approaches taken by the different groups
- Desert Tortoise: Phast results from all groups in good agreement with measurements (all predictions within a factor of two)
- FLADIS: Mixed results
  - DNV obtained good predictions using two-phase source from SMEDIS project (more than half predictions within a factor of two of measurements)
  - Other groups encountered issues: Phast simulated a vapour-phase release for FLADIS trials 9 and 24, due to specified exit temperature and pressure
  - Resulted in up to a factor of four difference between model predictions from different groups, and up to a factor of ten difference between predictions and measurements
- Causes of discrepancies were investigated
- The exercise provided valuable learning lessons for all involved
- Recommendations provided for how best to use Phast going forward for later JRIII work

Acknowledgements

- Sincere thanks to participants in the modelling exercise: Mike Harper and Frank Hart (DNV), Stephen Puttick and Adeel Ibrahim (Syngenta), Laurent Verdier (DGA) and Sandra Nilsen (Equinor)

Thank you

Any questions?

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