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

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

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

21st International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes

27-30 September 2022

Aims

- Run a model inter-comparison exercise to evaluate the performance of atmospheric dispersion models using data from previous ammonia release experiments
  - To understand the accuracy of models that may be used to design the Jack Rabbit III trials, e.g. to design the JRIII sensor array
  - To identify important model input parameters that we may need to carefully assess or measure in the trials

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)

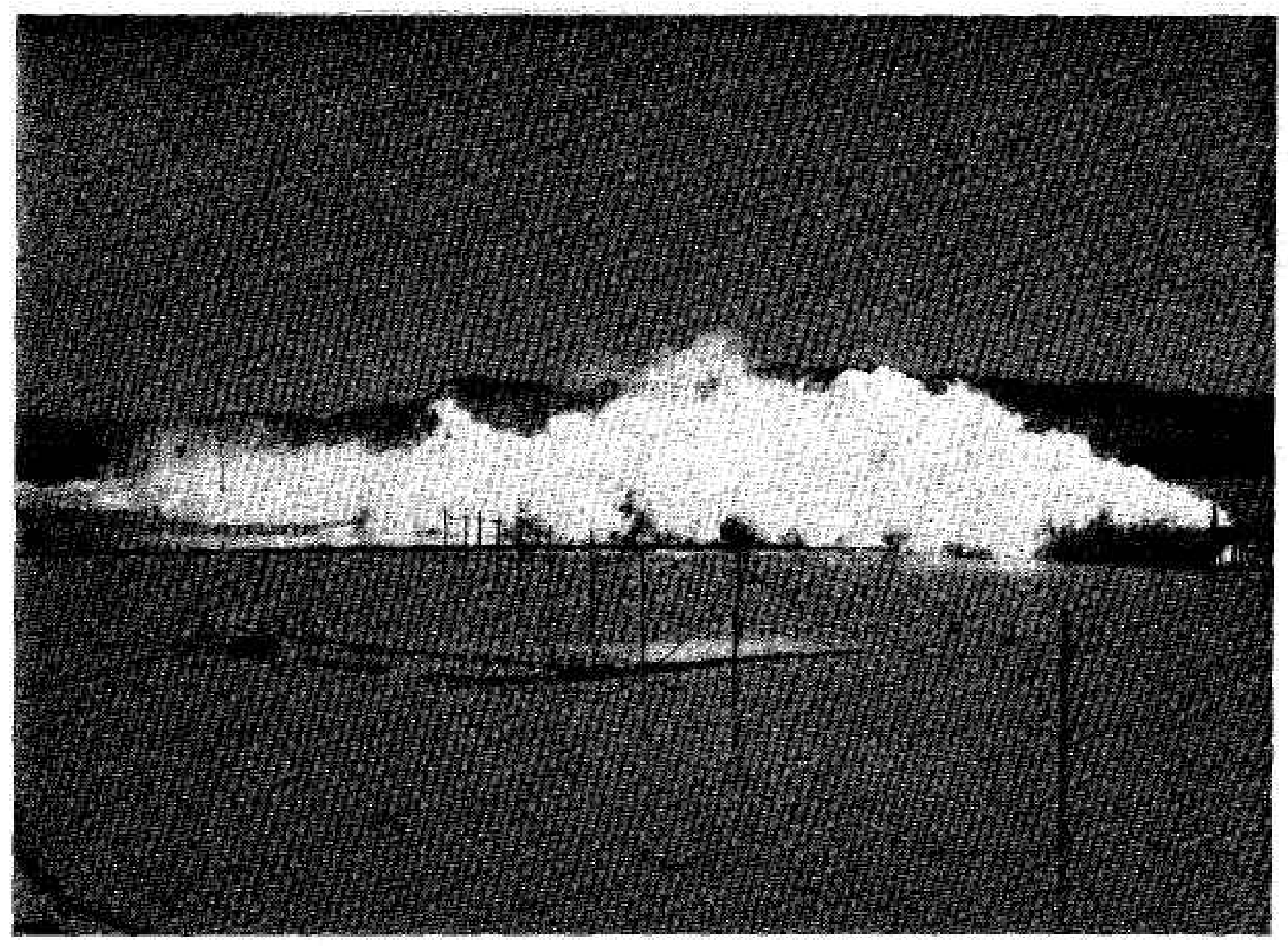

Fig. 15. Desert Tortoise 2 (upwind wide angle camera) Time = 230s. Lawrence Livermore National Laboratory

Methodology

- Participants provided with specified set of model inputs for Desert Tortoise and FLADIS
- Requested to provide basic set of model outputs (as a minimum)
  - Long time-averaged centerline plume concentrations for each of 6 trials
- Optionally, modelers can provide additional model outputs
  - E.g., predicted plume widths, temperatures, results from sensitivity tests
- Coordinators collated results, cross-plotted predictions against experimental measurements and shared results with participants
- Not a competition but a collaborative effort, with the ultimate goal of improving toxic industrial chemical modeling tools in general
- Timeline
  - Exercise initiated over Winter 2021-2022
  - Results shared with participants in Spring 2022
  - Concluded in Summer 2022 with aim to present findings at GMU conference

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Modeling Inputs

		DT1	DT2	DT4	FLADIS9	FLADIS16	FLADIS24
Orifice diameter	m	0.081[a]	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[b]	bara	10.1	11.2	11.8	6.93[c]	7.98[c]	5.70[c]
	barg	9.22	10.3	10.9	5.91	6.96	4.69
Release rate	kg/s	80.0[d]	117[e]	108[f]	0.40	0.27	0.46
Release duration	s	126	255	381	900	1200[g]	600
Site average wind speed	m/s	7.42	5.76	4.51[h]	6.1[i]	4.4	4.9[j]
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[k]	D	D-E	C-D[l]
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

- All trials involved horizontal releases of pressure-liquefied ammonia over flat, unobstructed terrain
- Data taken primarily from SMEDIS database (https://admlc.com/smedis-dataset)
- Cross-checks carried out with other information sources
  - Modelers Data Archive
  - REDIPHEM
  - Original data reports, e.g. Goldwire *et al*. (1985)
  - Notes provided to explain choice of values

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Participants in the JRIII 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		■			■	■	■	■	■	■

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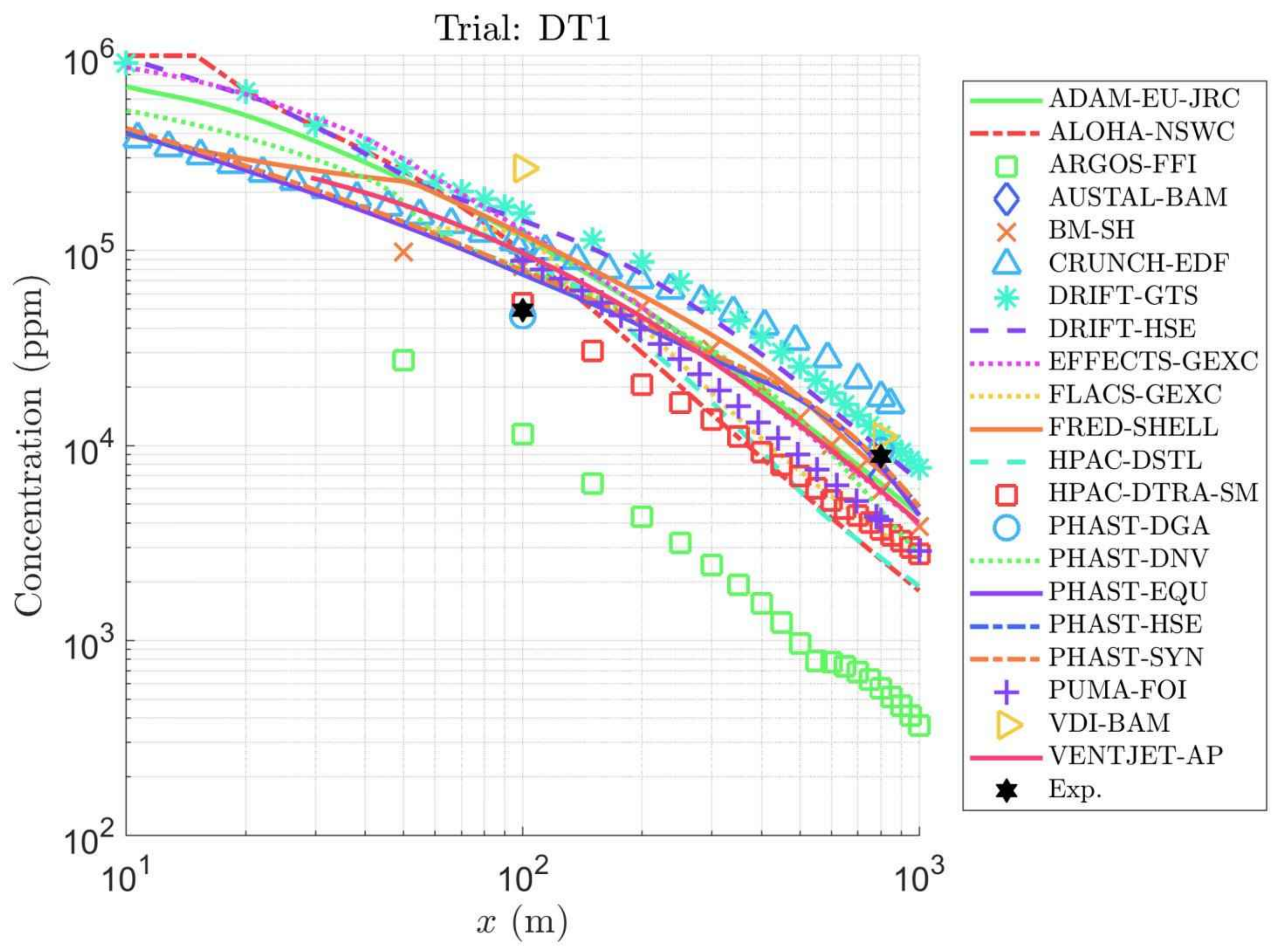
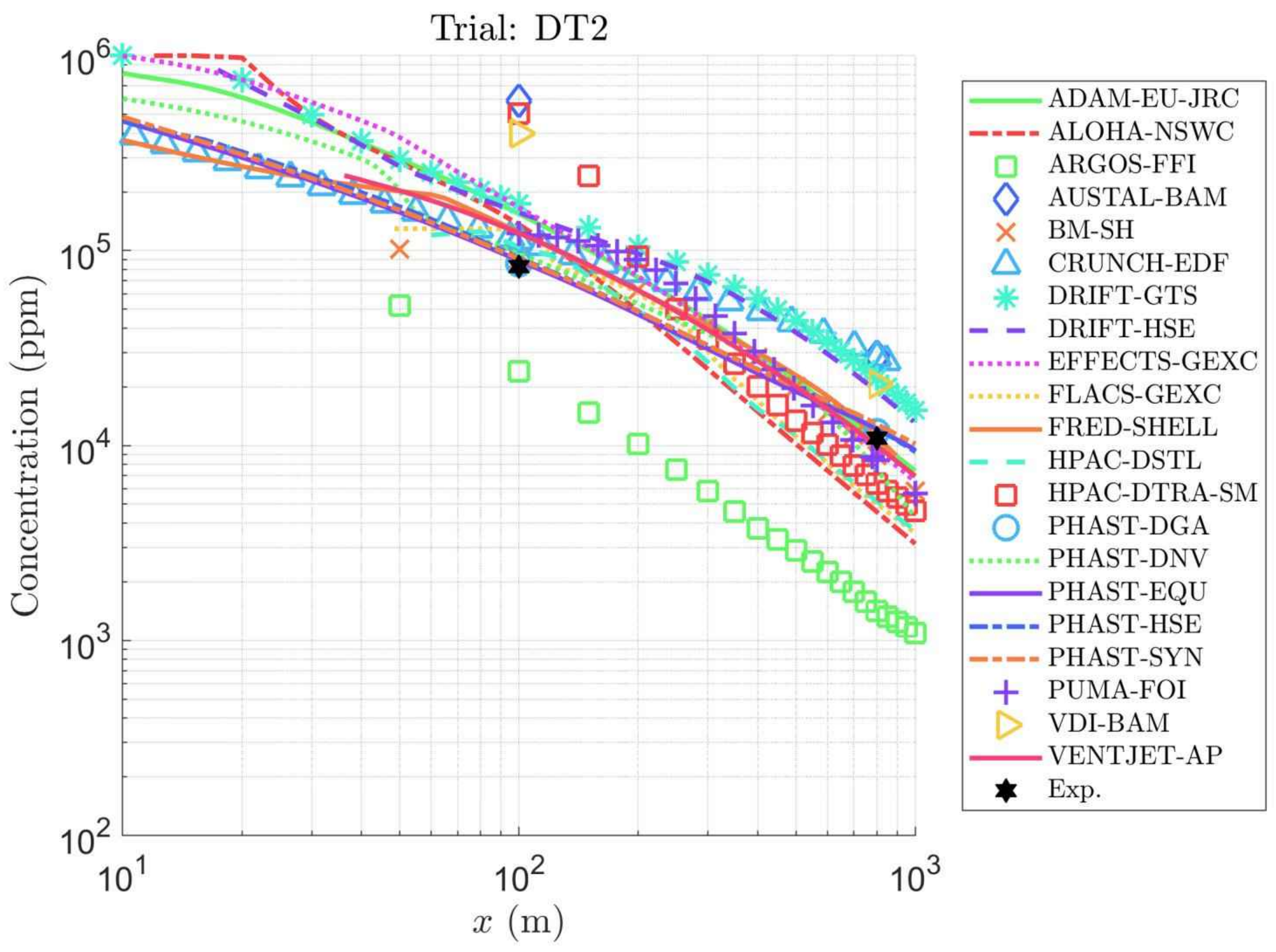
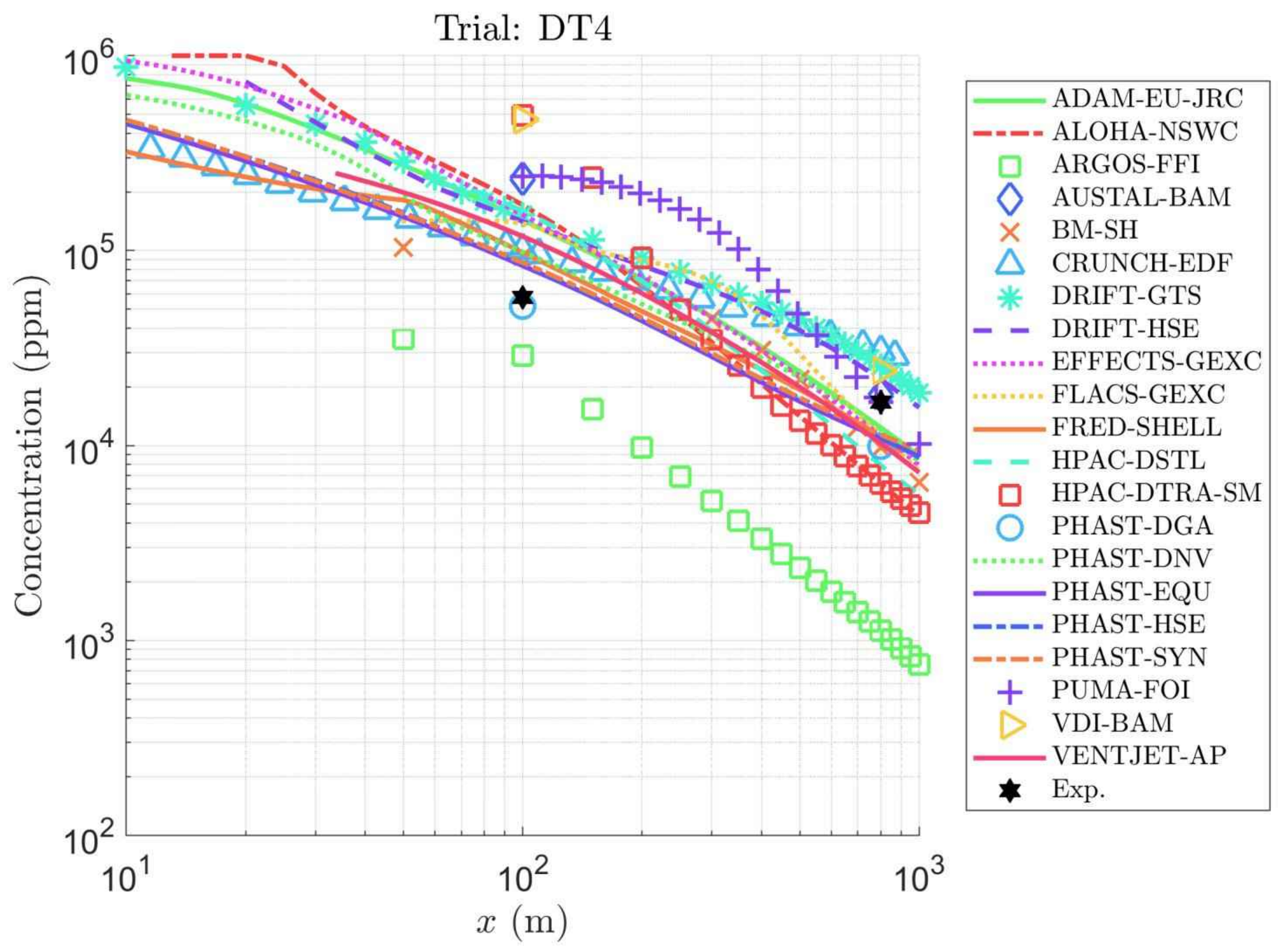
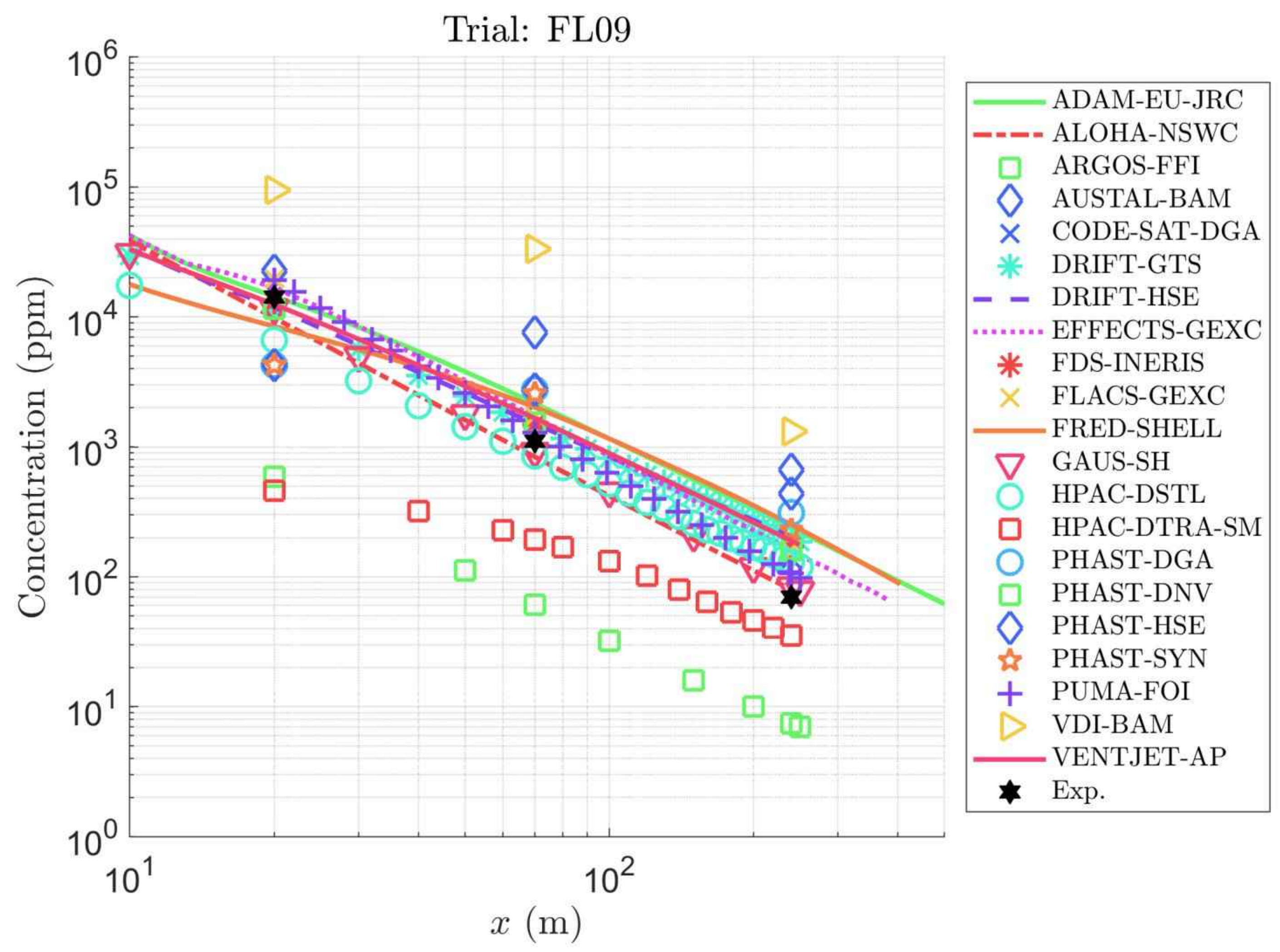
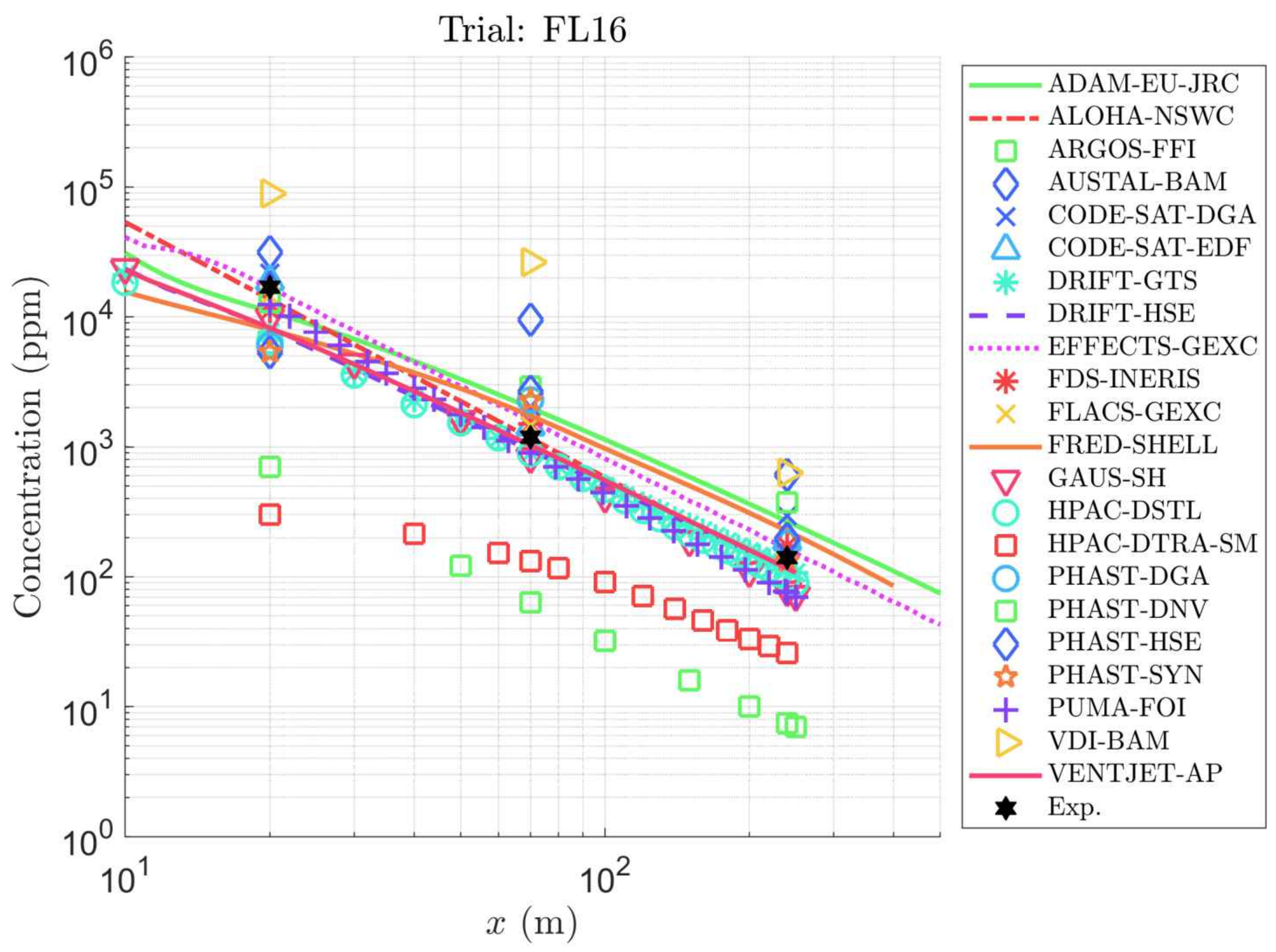
All Model Results

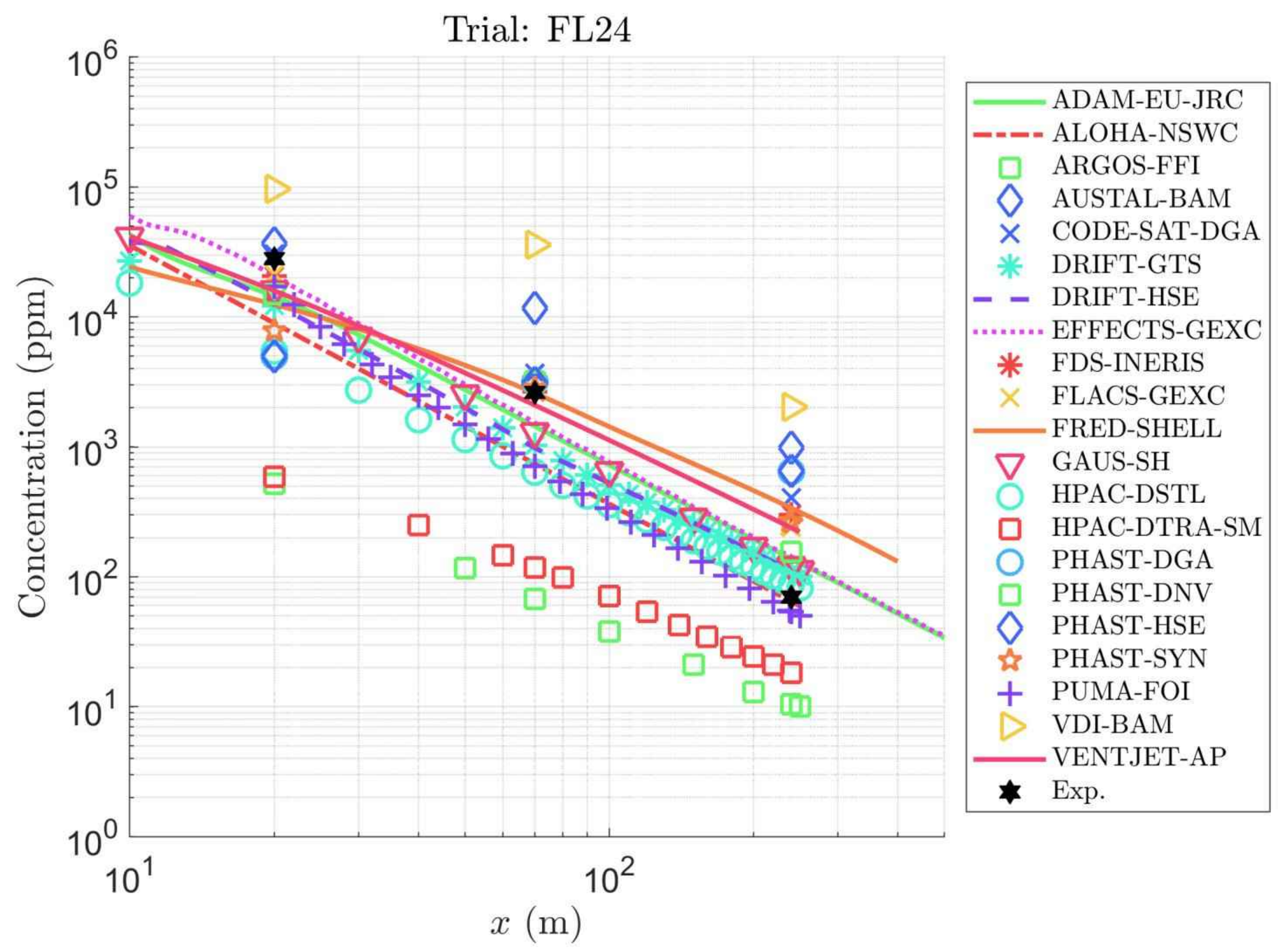












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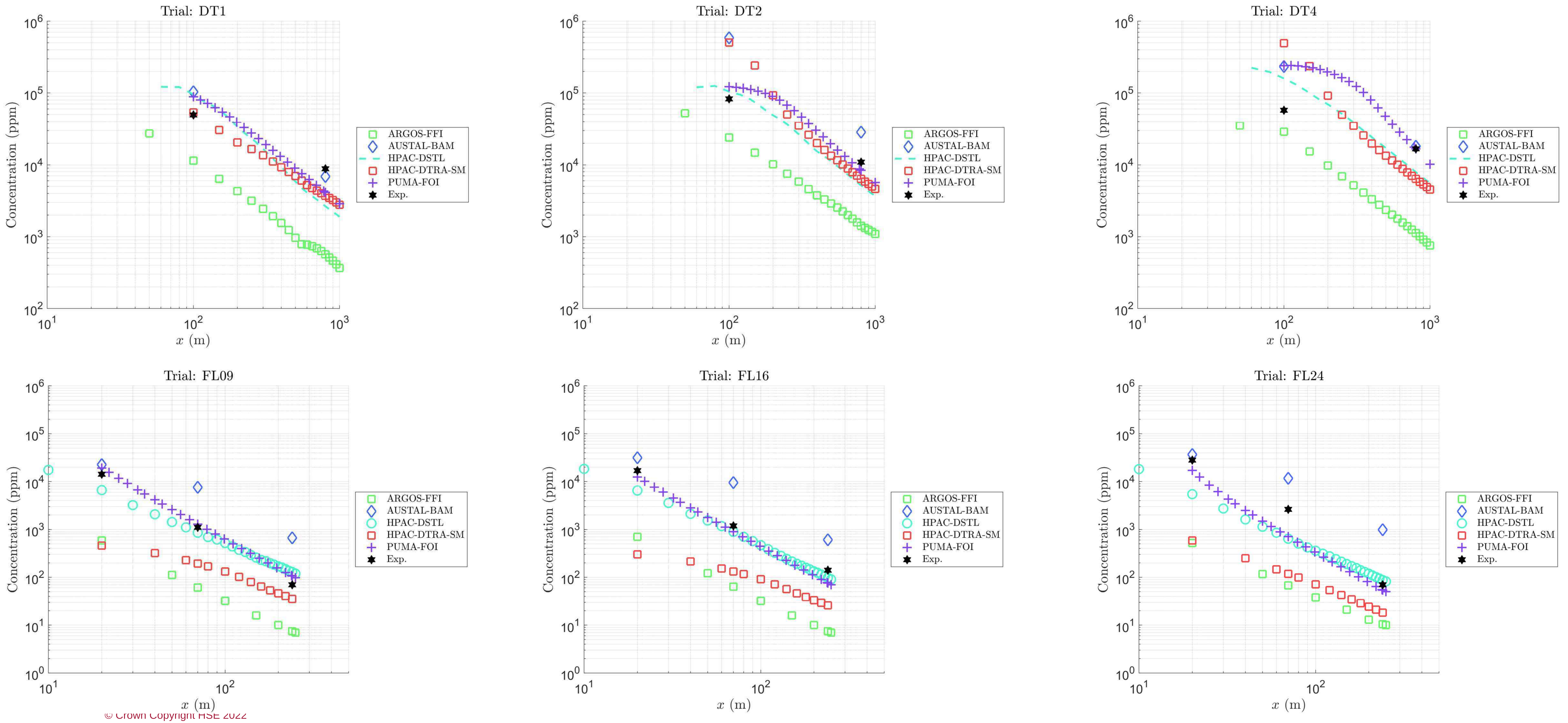
Gaussian Puff, Lagrangian



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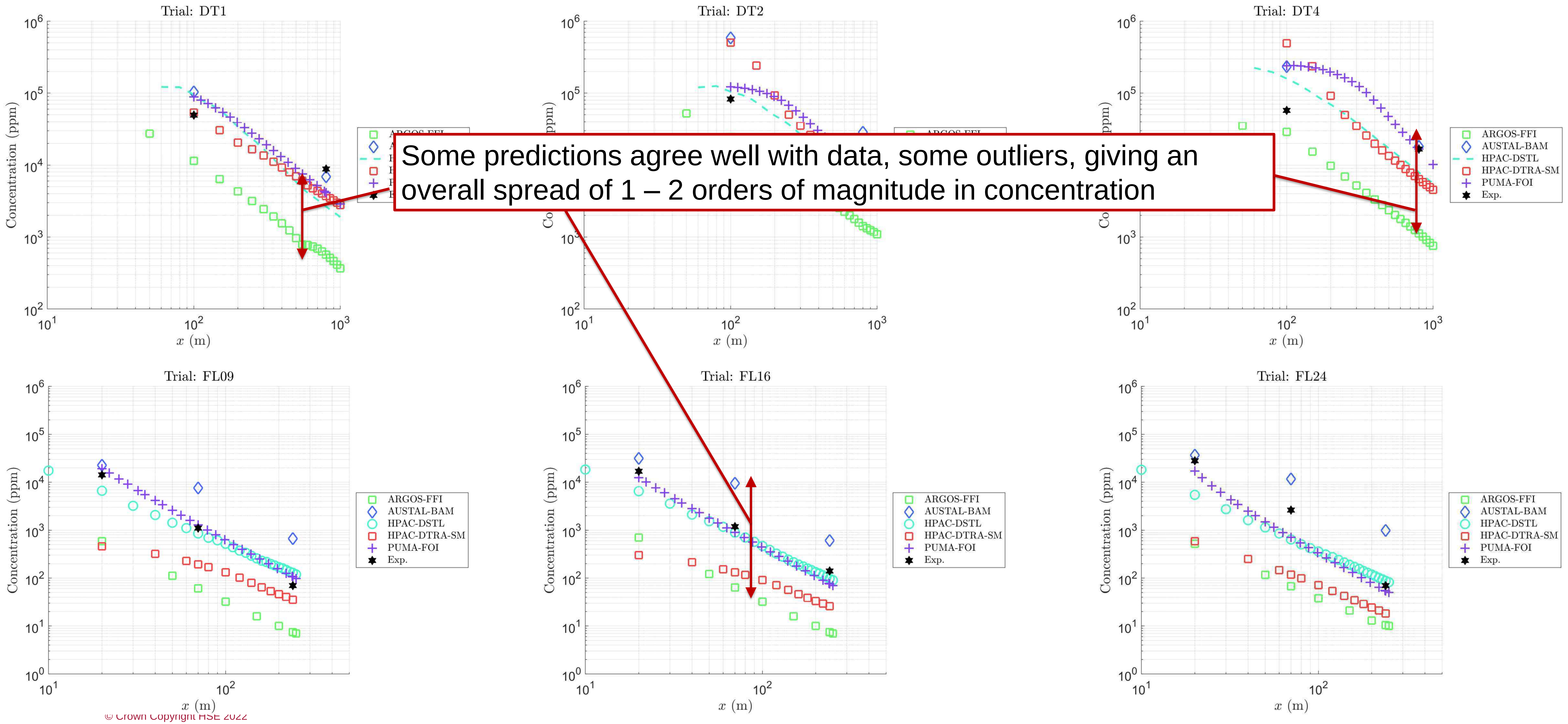
Gaussian Puff, Lagrangian



Some predictions agree well with data, some outliers, giving an overall spread of 1 – 2 orders of magnitude in concentration

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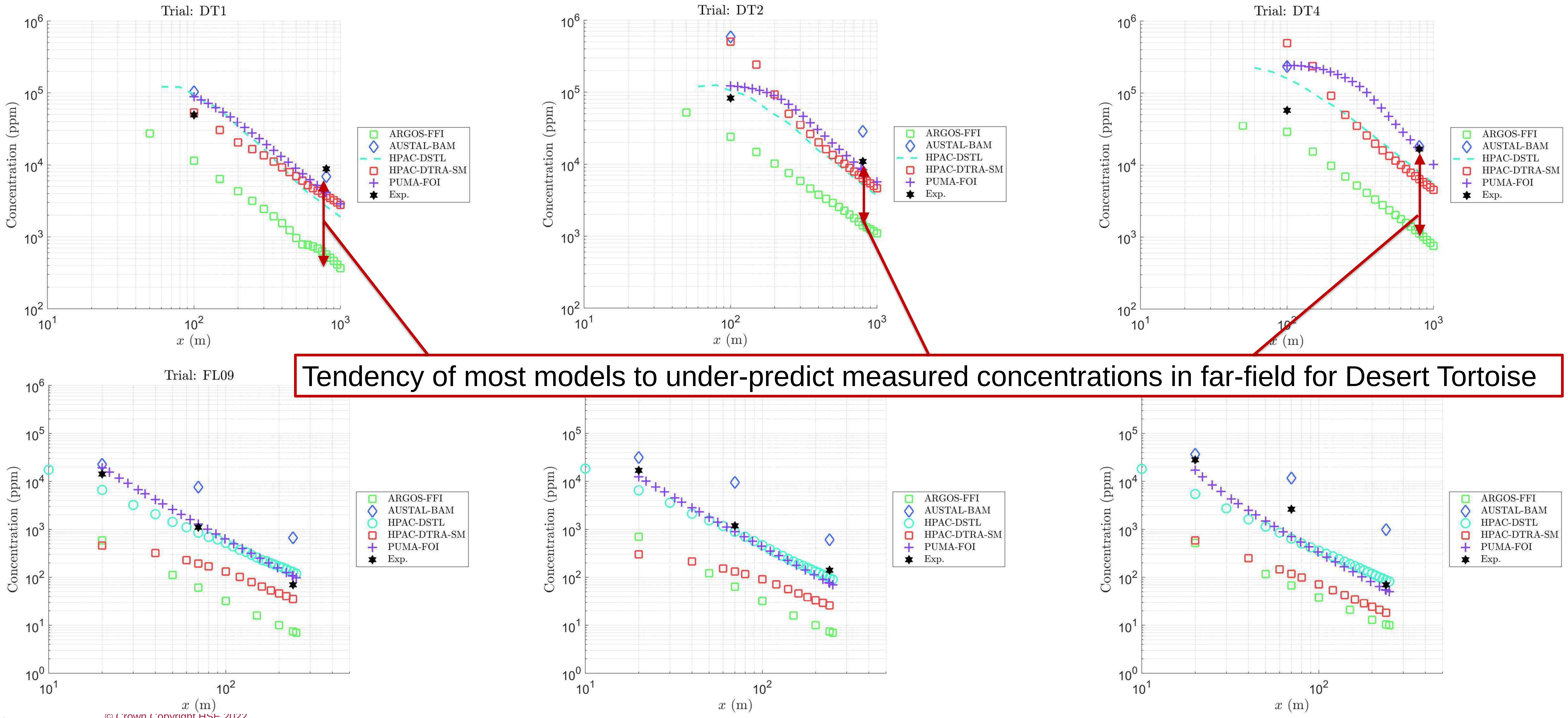
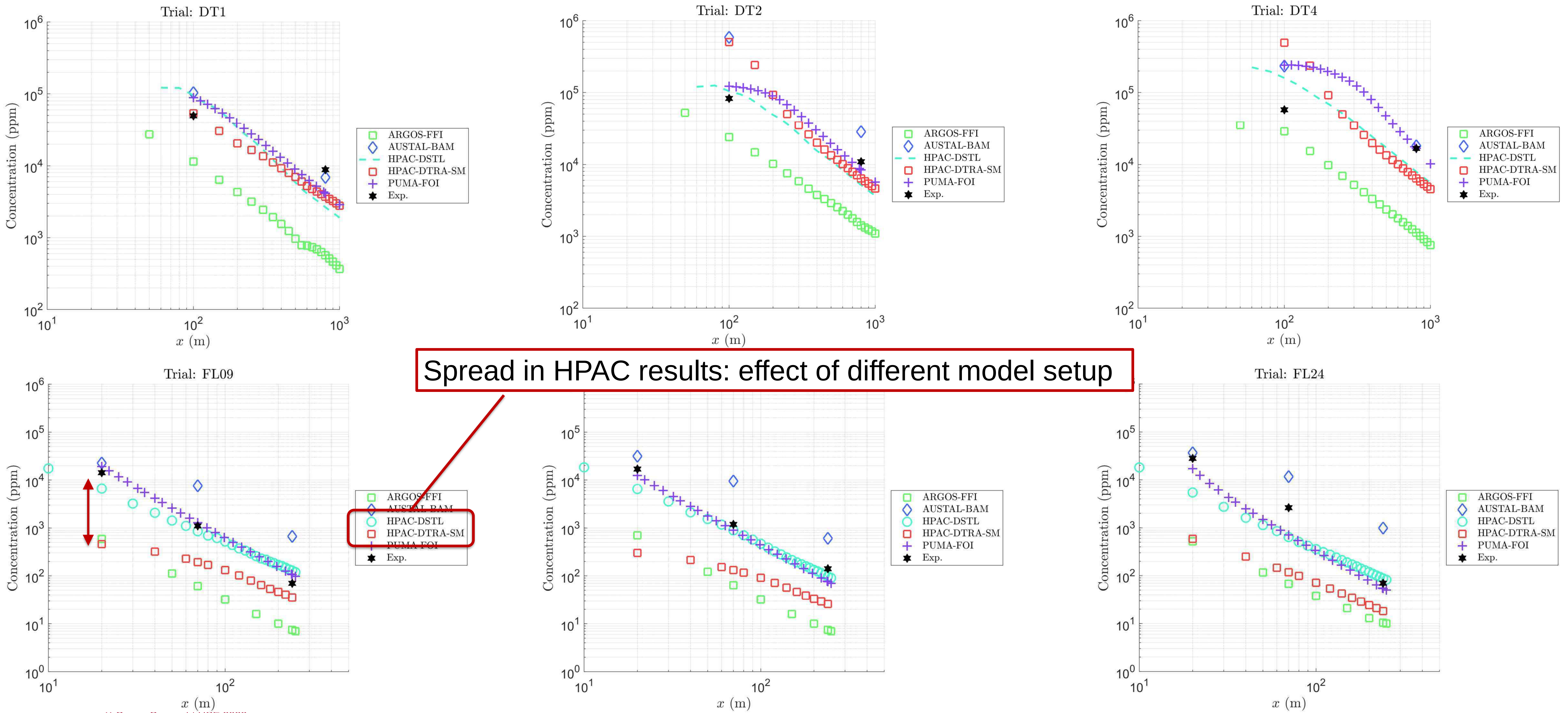
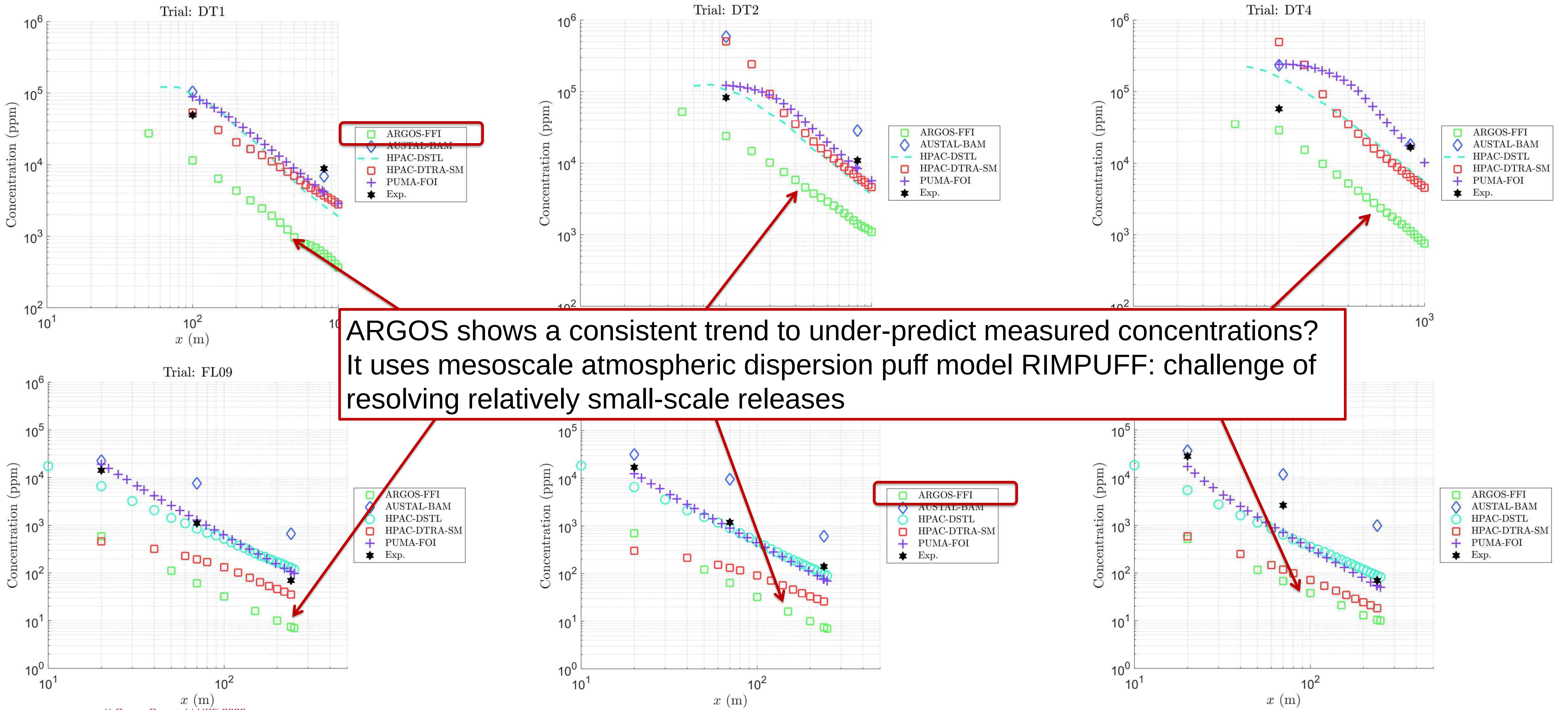
Gaussian Puff, Lagrangian



Gaussian Puff, Lagrangian

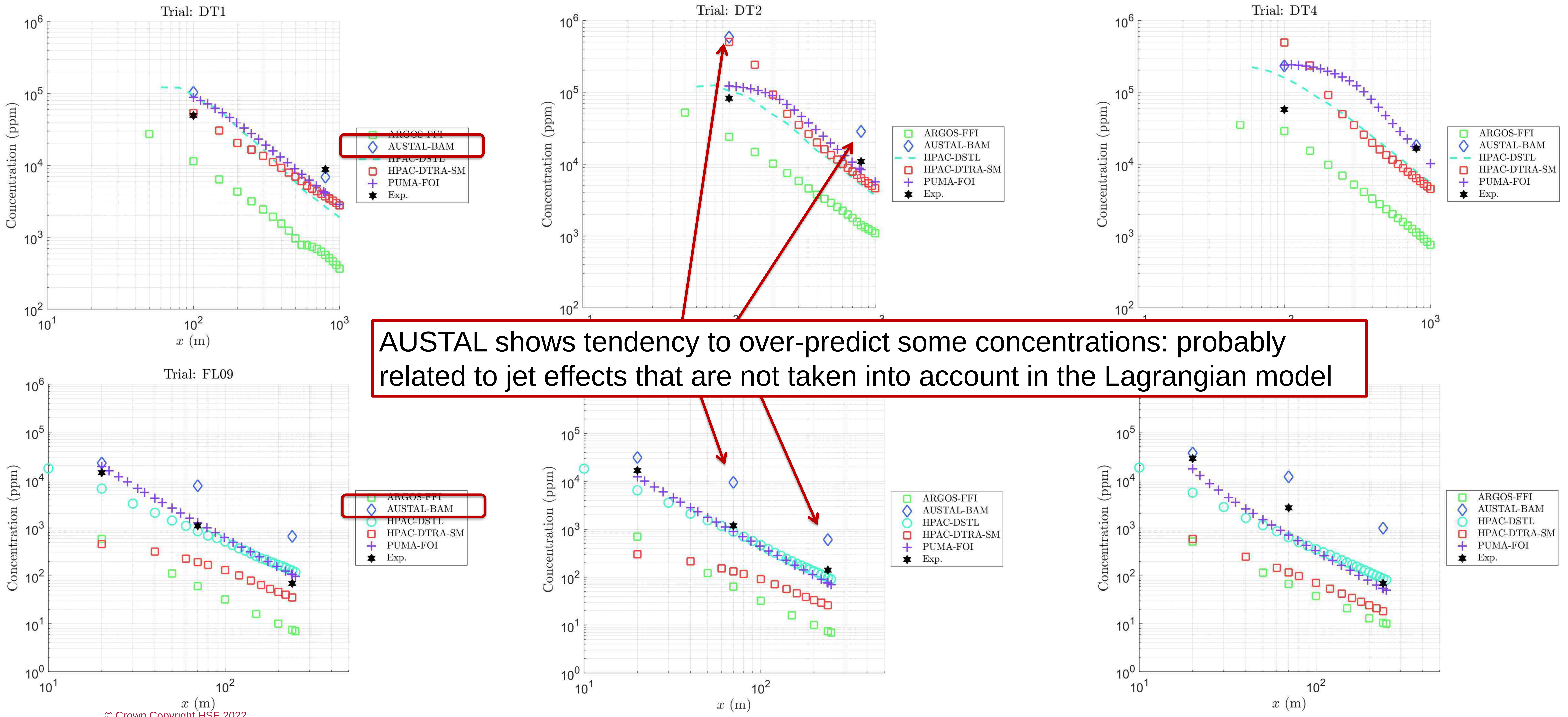


Gaussian Puff, Lagrangian



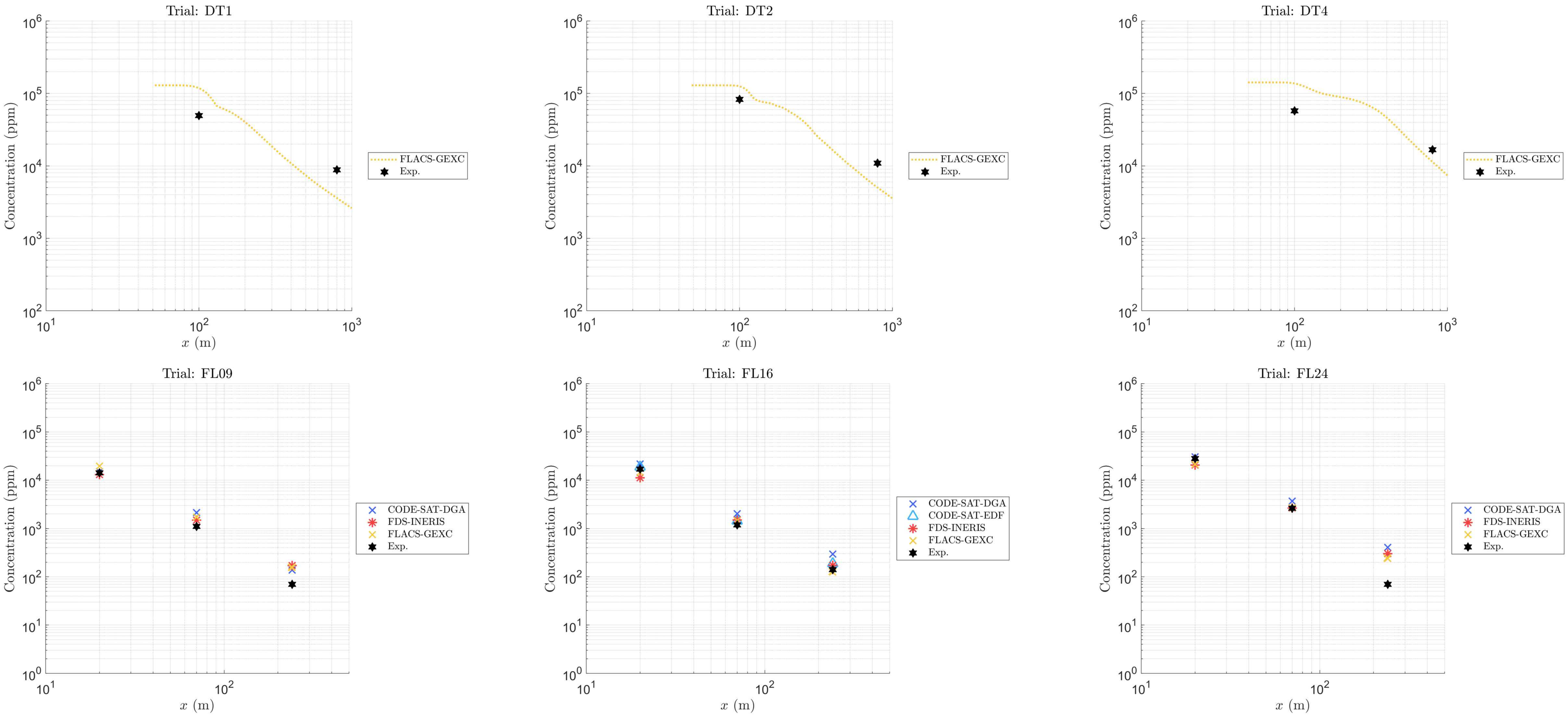
ARGOS shows a consistent trend to under-predict measured concentrations? It uses mesoscale atmospheric dispersion puff model RIMPUFF: challenge of resolving relatively small-scale releases

Gaussian Puff, Lagrangian



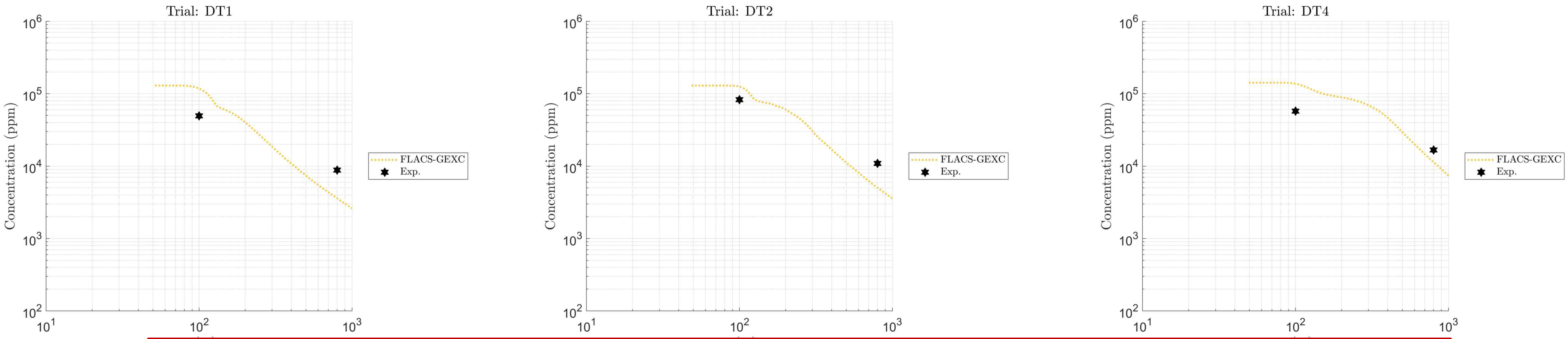
AUSTAL shows tendency to over-predict some concentrations: probably related to jet effects that are not taken into account in the Lagrangian model

CFD

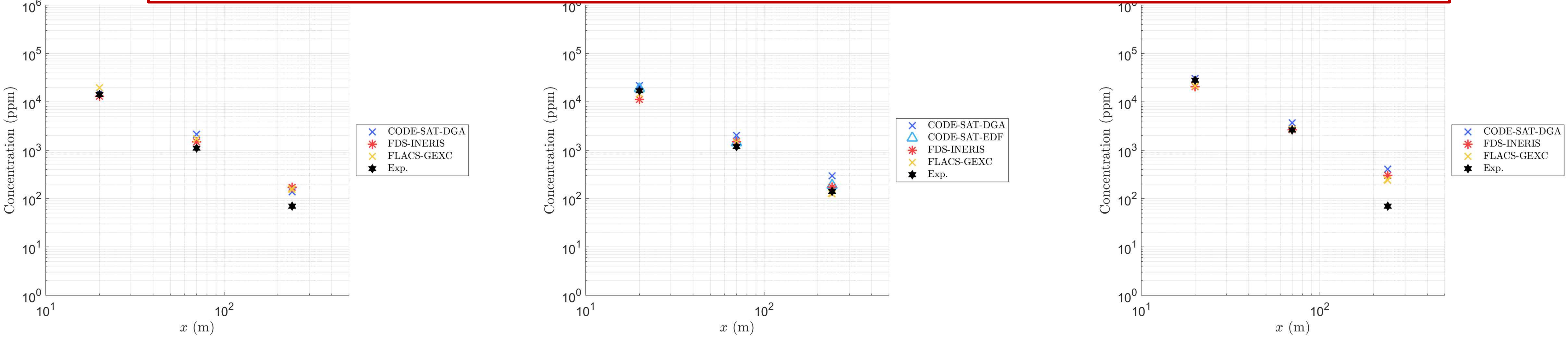


Trial: DT1
Concentration (ppm)
x (m)
FLACS-GEXC
Exp.
Trial: DT2
Concentration (ppm)
x (m)
FLACS-GEXC
Exp.
Trial: DT4
Concentration (ppm)
x (m)
FLACS-GEXC
Exp.
Trial: FL09
Concentration (ppm)
x (m)
CODE-SAT-DGA
FDS-INERIS
FLACS-GEXC
Exp.
Trial: FL16
Concentration (ppm)
x (m)
CODE-SAT-DGA
CODE-SAT-EDF
FDS-INERIS
FLACS-GEXC
Exp.
Trial: FL24
Concentration (ppm)
x (m)
CODE-SAT-DGA
FDS-INERIS
FLACS-GEXC
Exp.

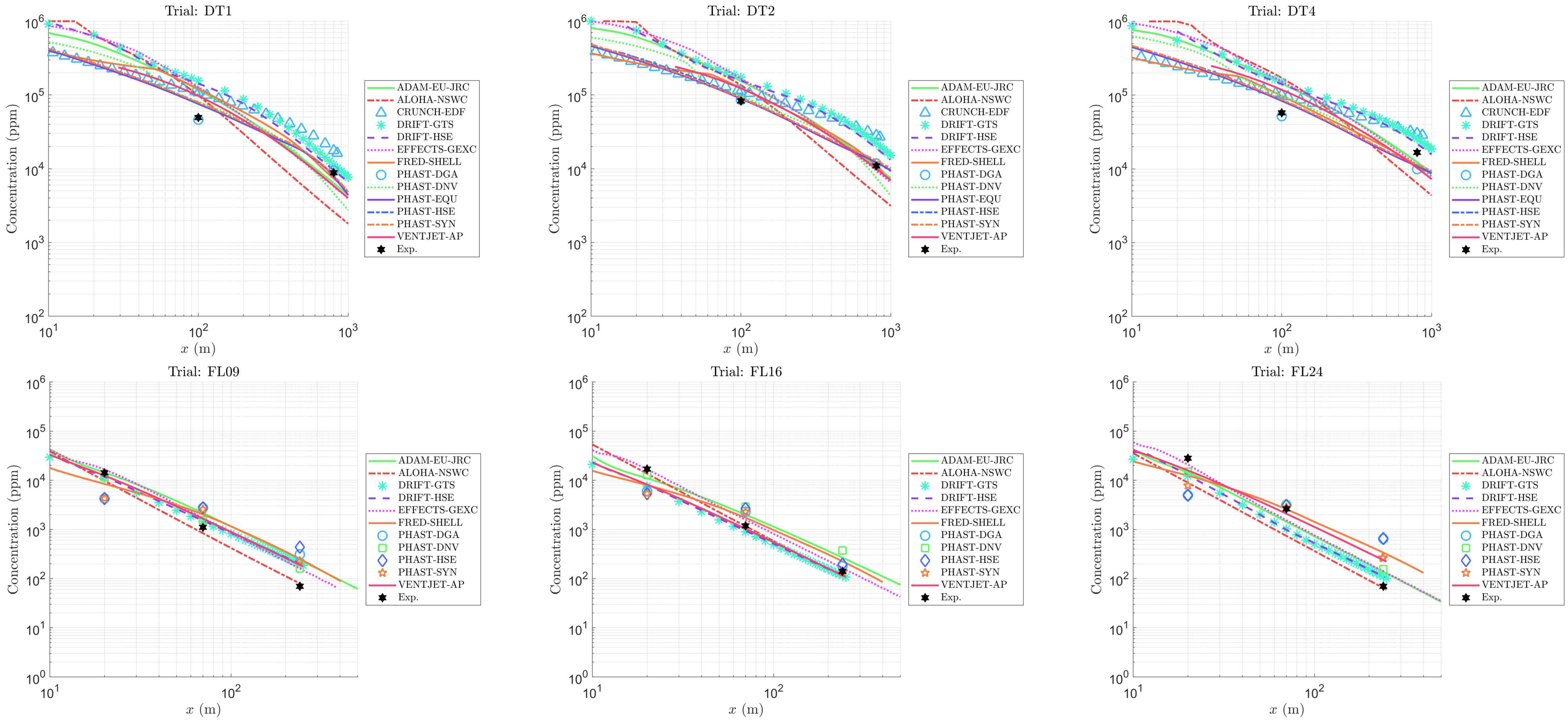
CFD



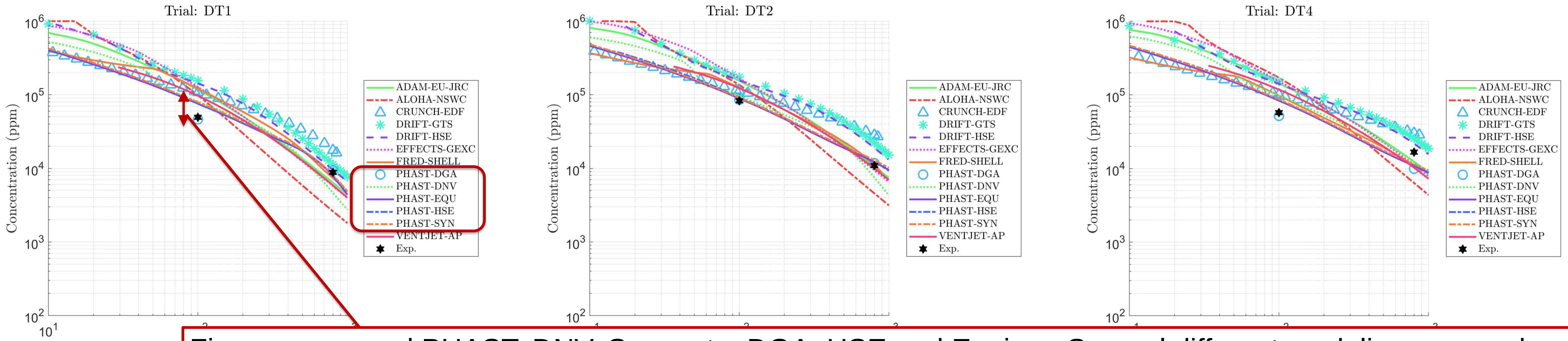
CFD models give remarkably similar results despite fundamentally different modeling approaches



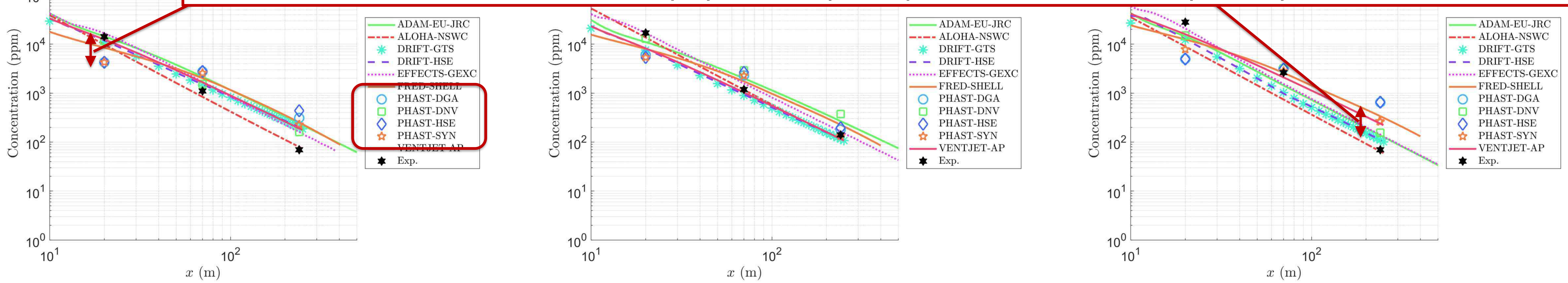
Integral


Trial: DT1
Trial: DT2
Trial: DT4
Trial: FL09
Trial: FL16
Trial: FL24
Concentration (ppm)
x (m)
ADAM-EU-JRC
ALOHA-NSWC
CRUNCH-EDF
DRIFT-GTS
DRIFT-HSE
EFFECTS-GEXC
FRED-SHELL
PHAST-DGA
PHAST-DNV
PHAST-EQU
PHAST-HSE
PHAST-SYN
VENTJET-AP
Exp.

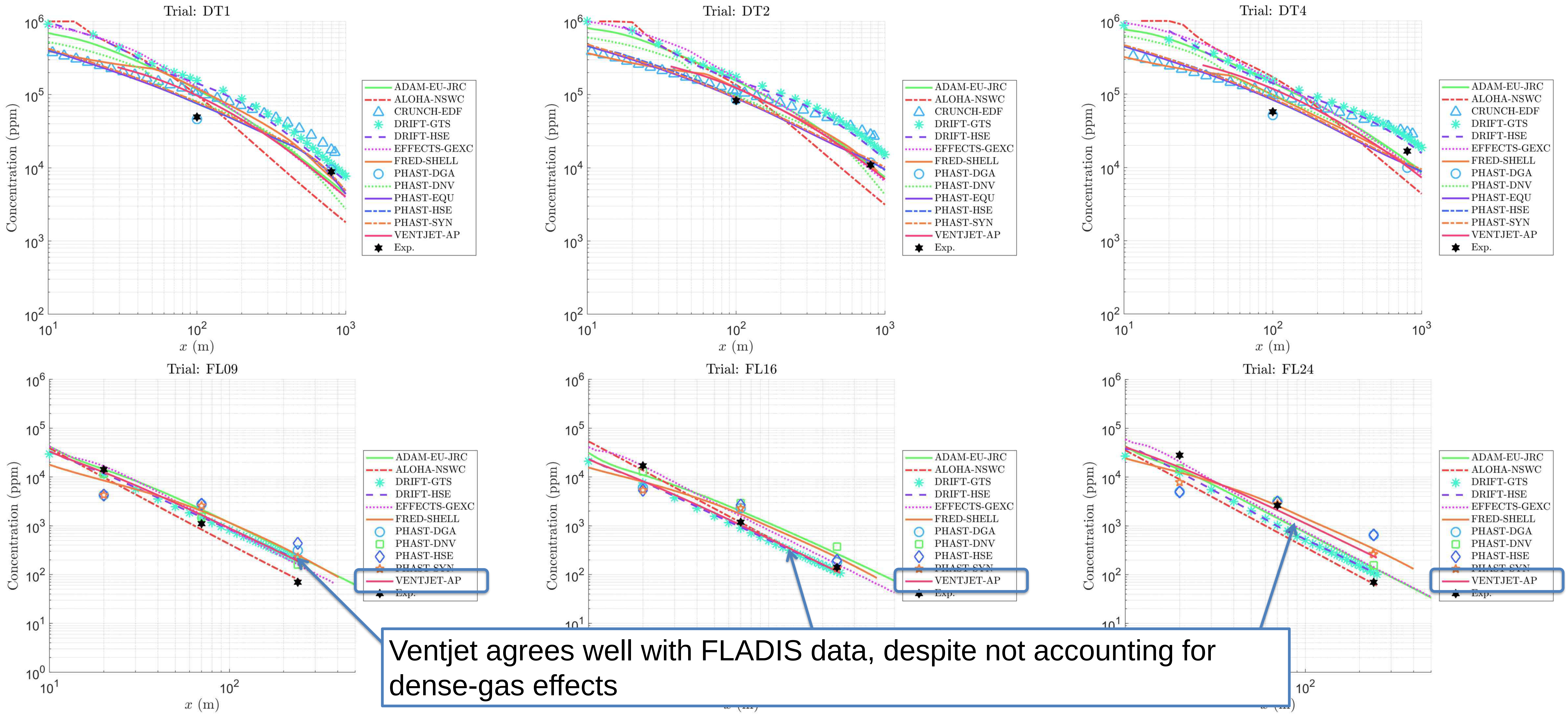
Integral



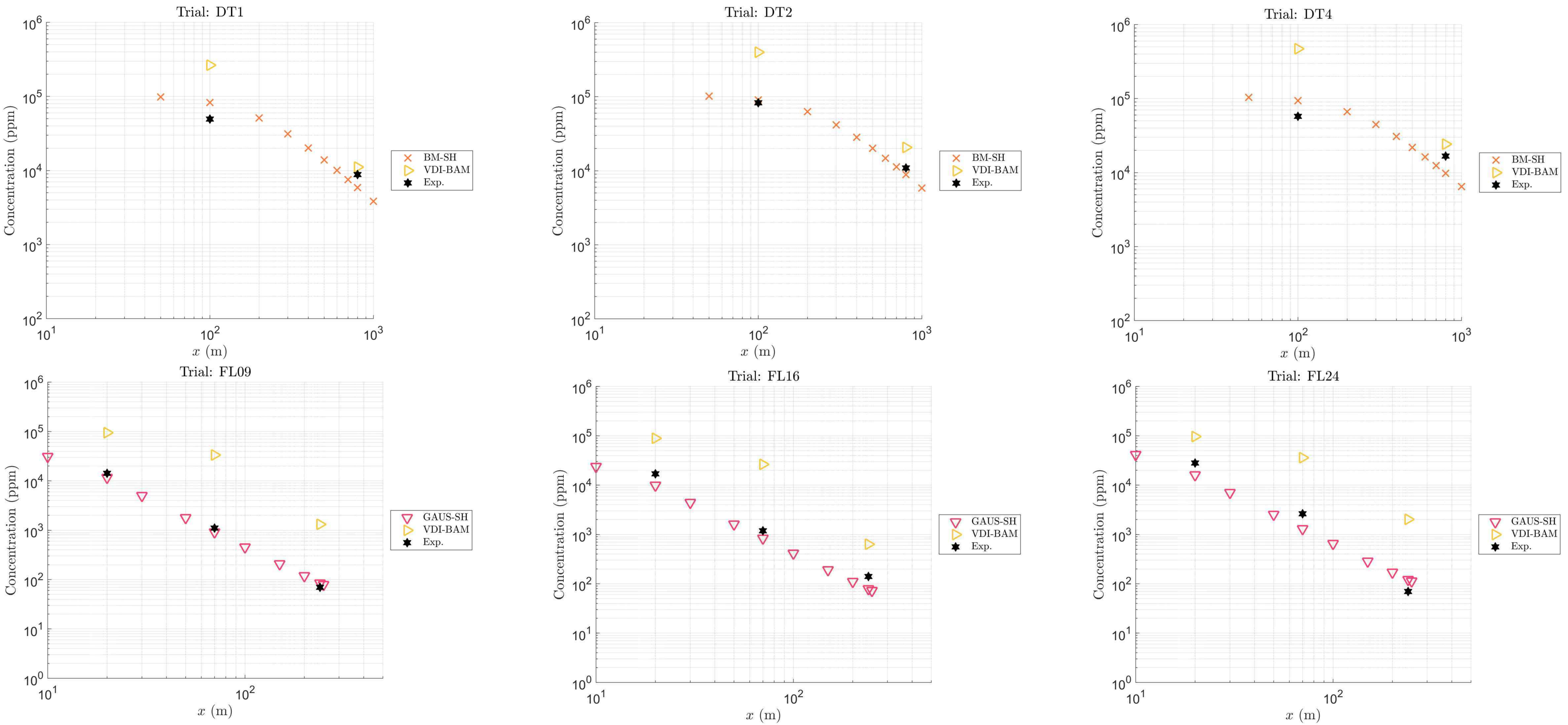
Five groups used PHAST: DNV, Syngenta, DGA, HSE and Equinor. Several different modeling approaches taken, some differences of factor of two (DT) to ten (FLADIS) when compared to measurements. Main differences due to source conditions (vapour/two-phase). Further details in separate presentation.



Integral


Trial: DT1
Trial: DT2
Trial: DT4
Trial: FL09
Trial: FL16
Trial: FL24
Concentration (ppm)
x (m)
ADAM-EU-JRC
ALOHA-NSWC
CRUNCH-EDF
DRIFT-GTS
DRIFT-HSE
EFFECTS-GEXC
FRED-SHELL
PHAST-DGA
PHAST-DNV
PHAST-EQU
PHAST-HSE
PHAST-SYN
VENTJET-AP
Exp.
Ventjet agrees well with FLADIS data, despite not accounting for dense-gas effects

Empirical Nomograms, Gaussian Plume



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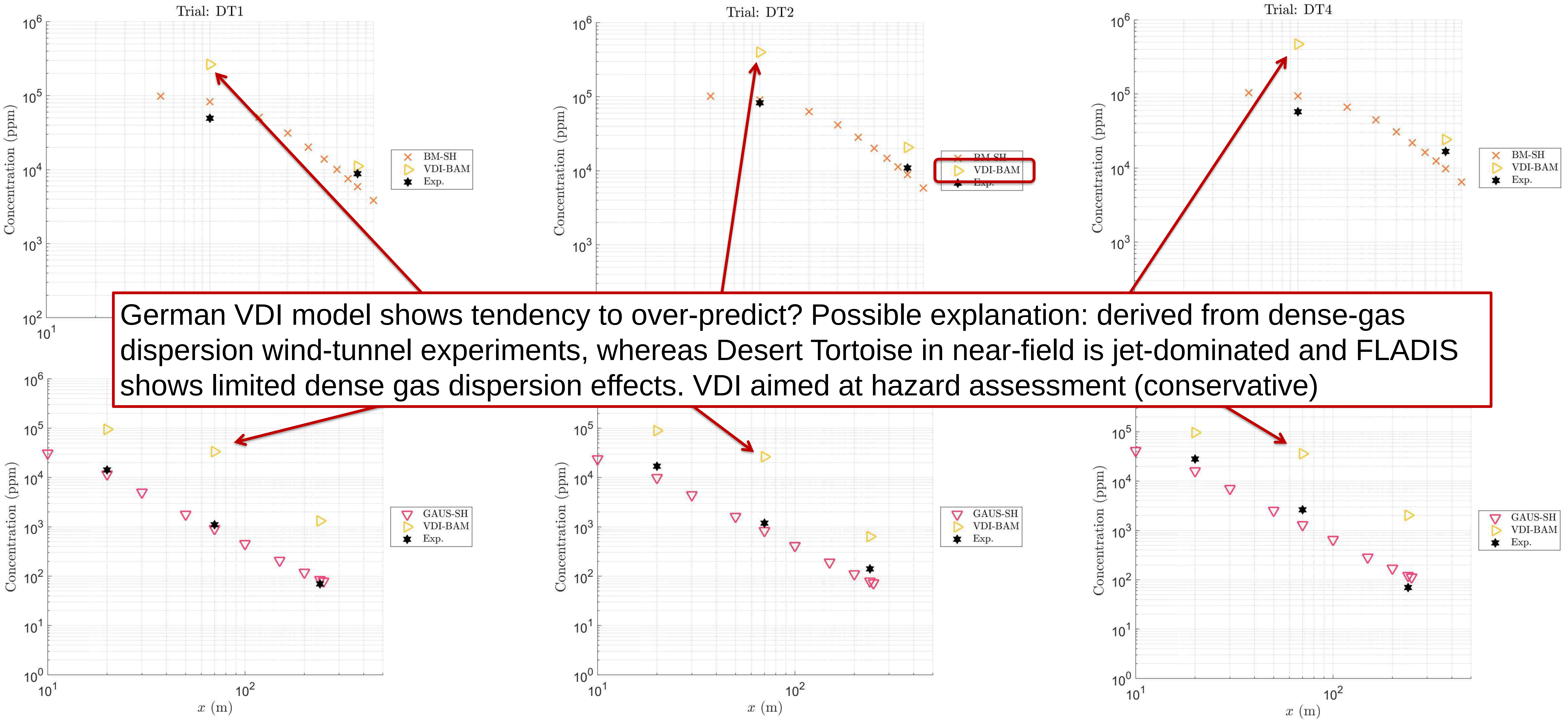
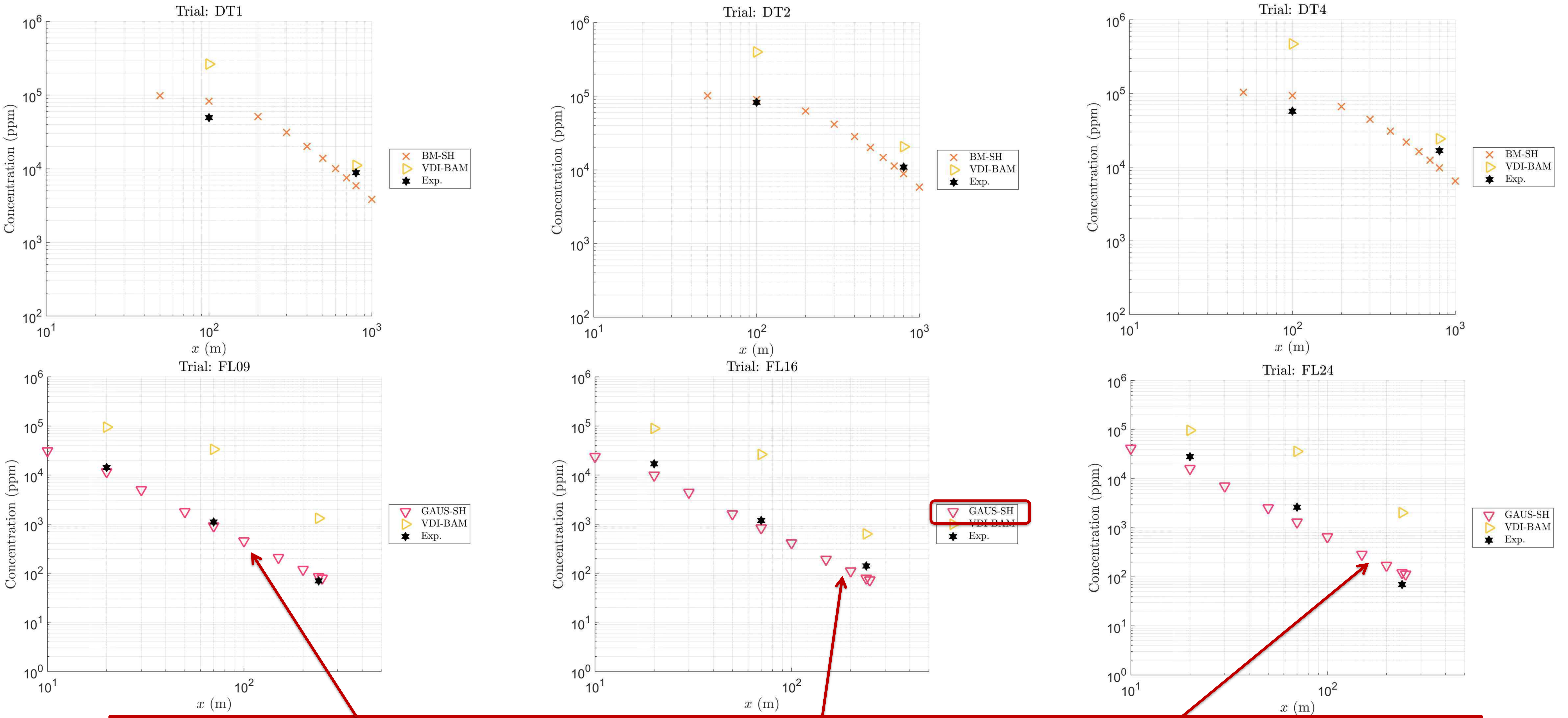
Empirical Nomograms, Gaussian Plume



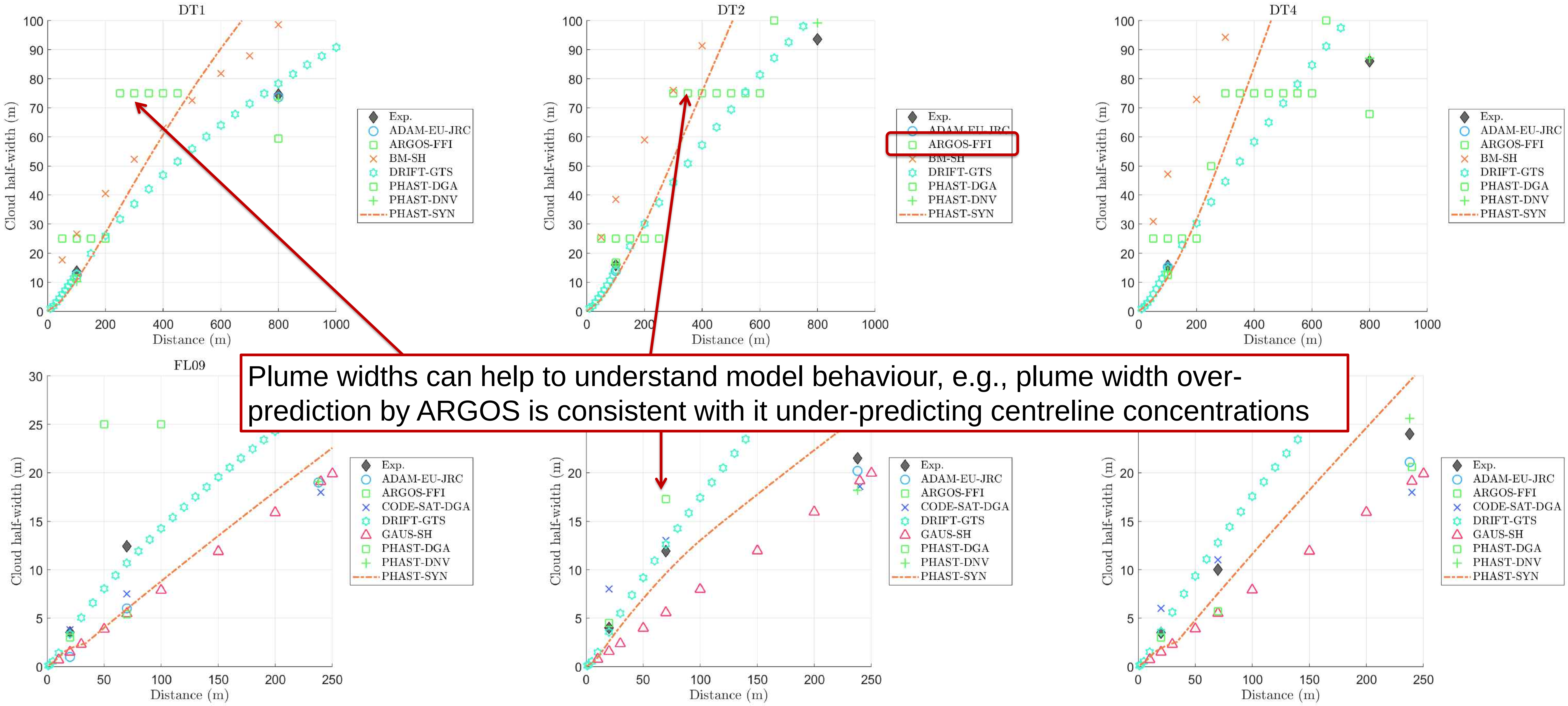
German VDI model shows tendency to over-predict? Possible explanation: derived from dense-gas dispersion wind-tunnel experiments, whereas Desert Tortoise in near-field is jet-dominated and FLADIS shows limited dense gas dispersion effects. VDI aimed at hazard assessment (conservative)

Empirical Nomograms, Gaussian Plume



Gaussian plume model agrees well with FLADIS data, despite not accounting for dense-gas effects

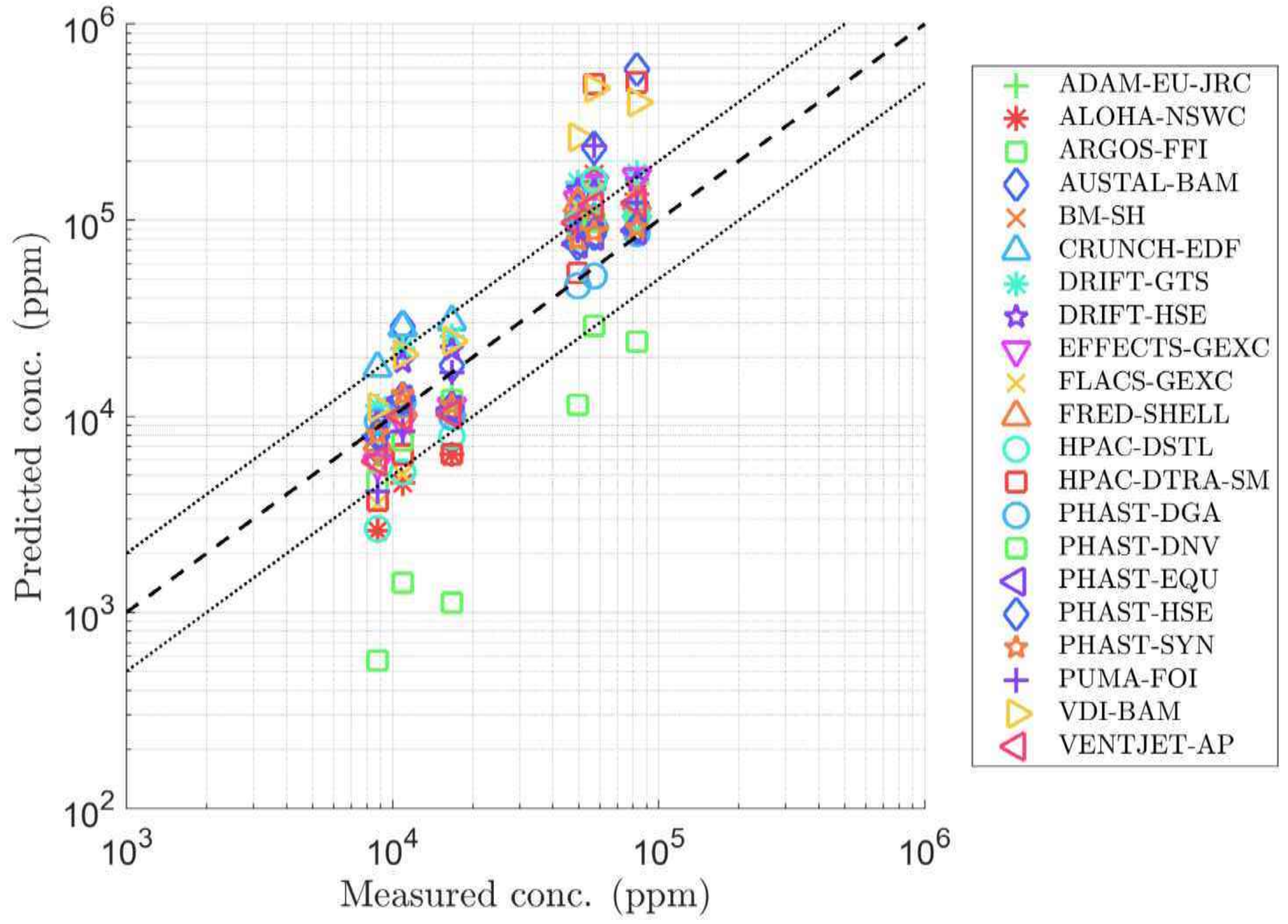
Plume Half-Widths



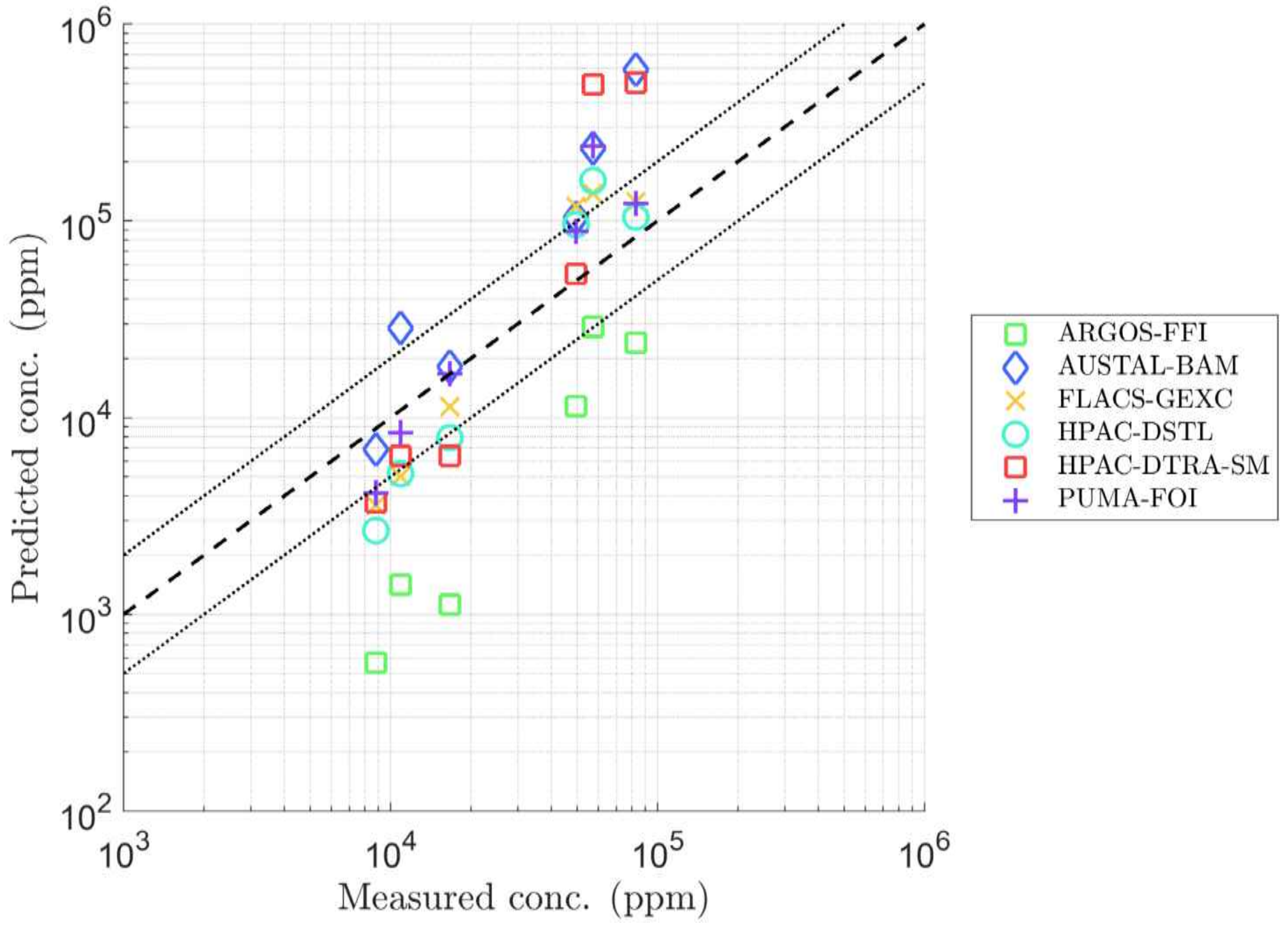
Plume widths can help to understand model behaviour, e.g., plume width over-prediction by ARGOS is consistent with it under-predicting centreline concentrations

Desert Tortoise

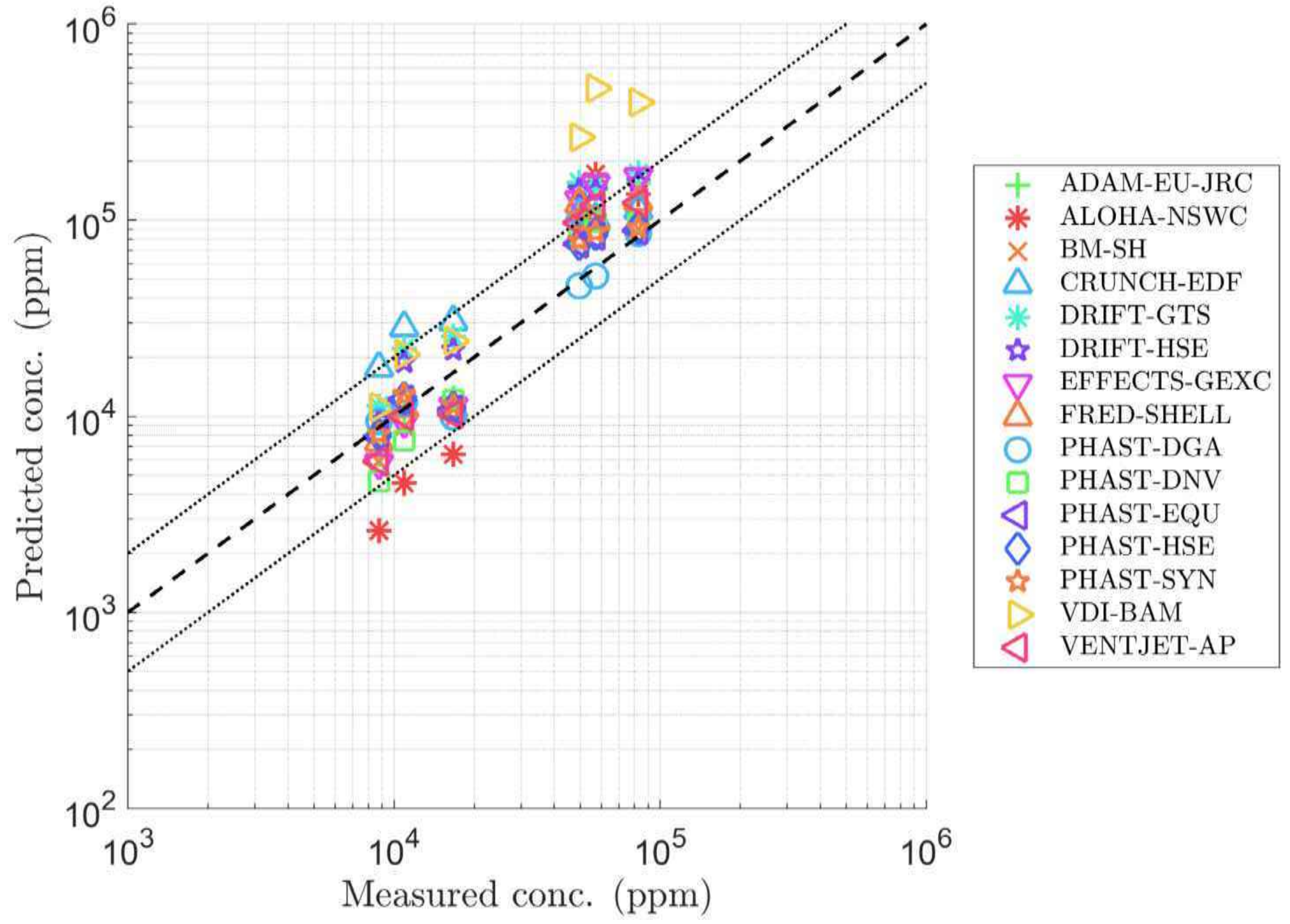
Predicted versus Measured Centerline Concentrations



All results



CFD, Gaussian puff, Lagrangian



Empirically-based nomograms, integral, Gaussian plume

Desert Tortoise

Predicted versus Measured Centerline Concentrations

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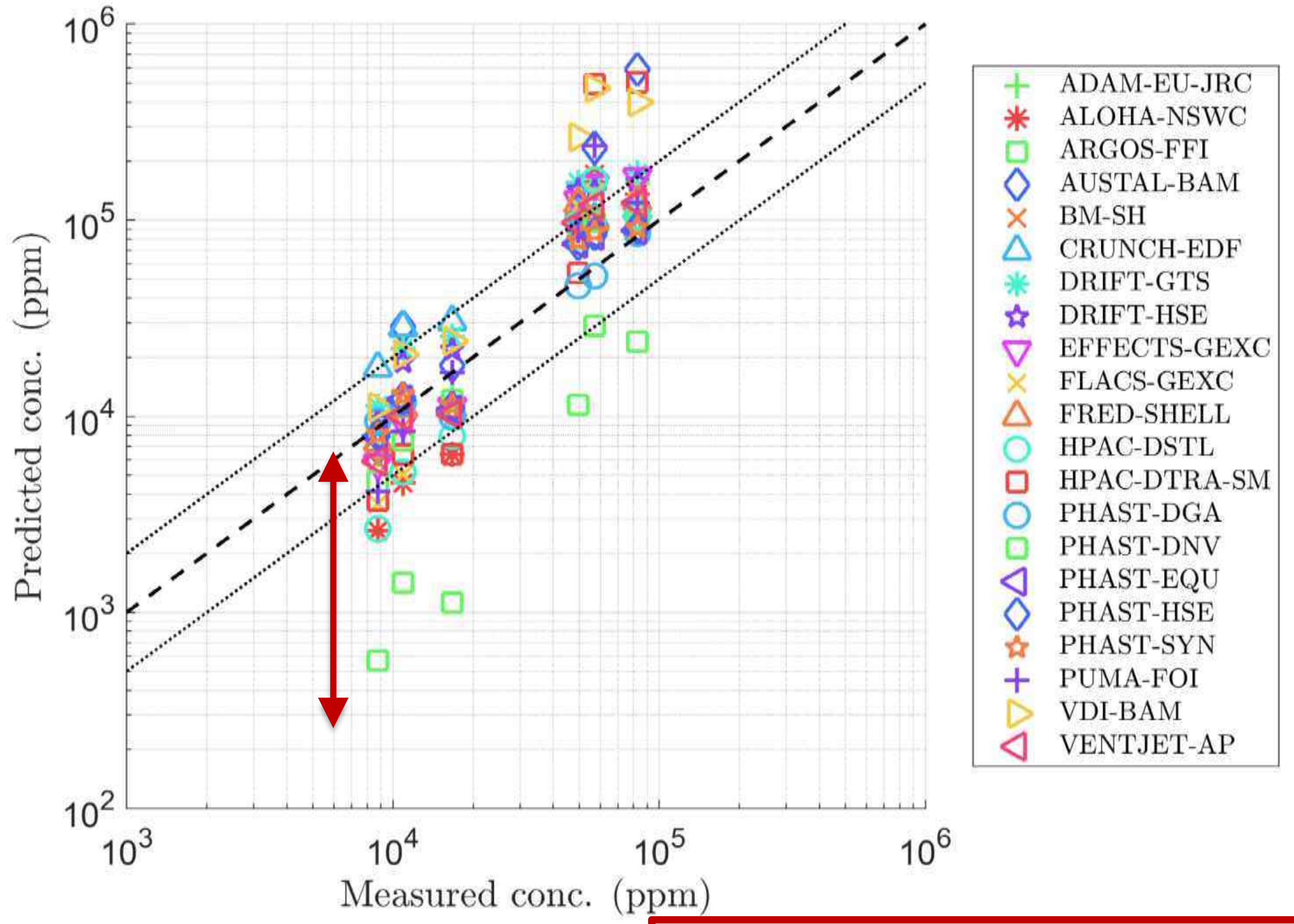
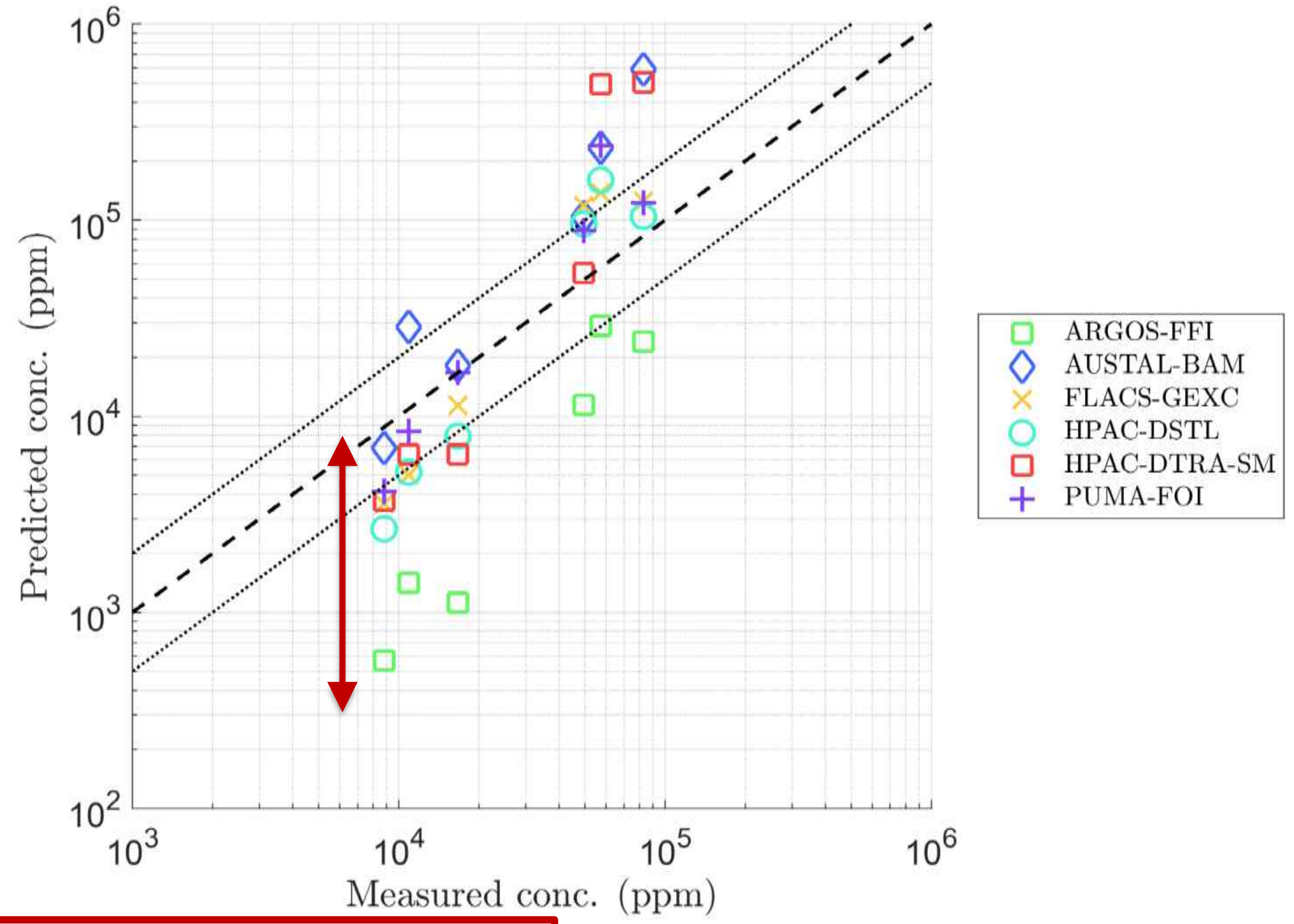
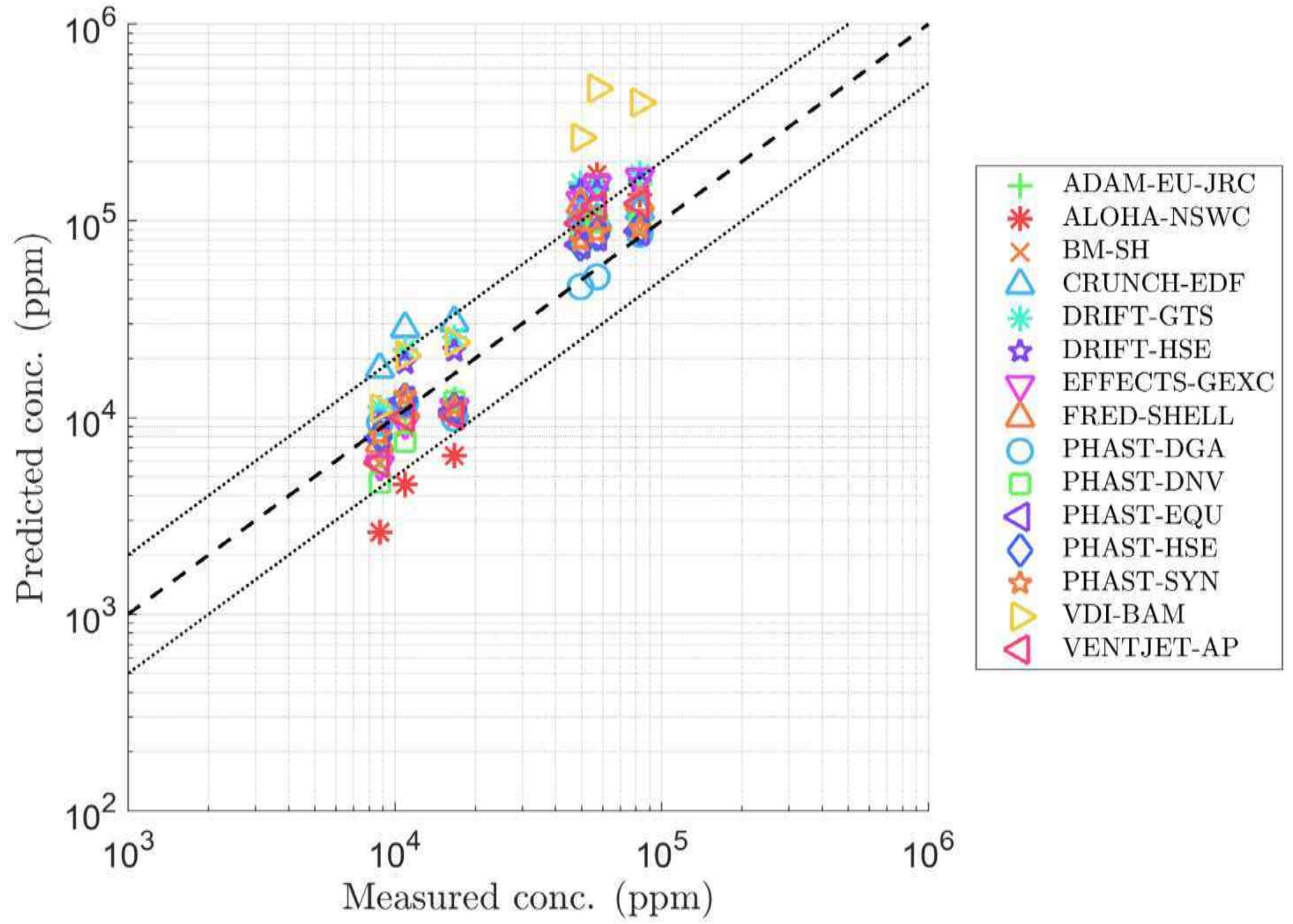






Trend towards under-predicting far field concentrations in Desert Tortoise

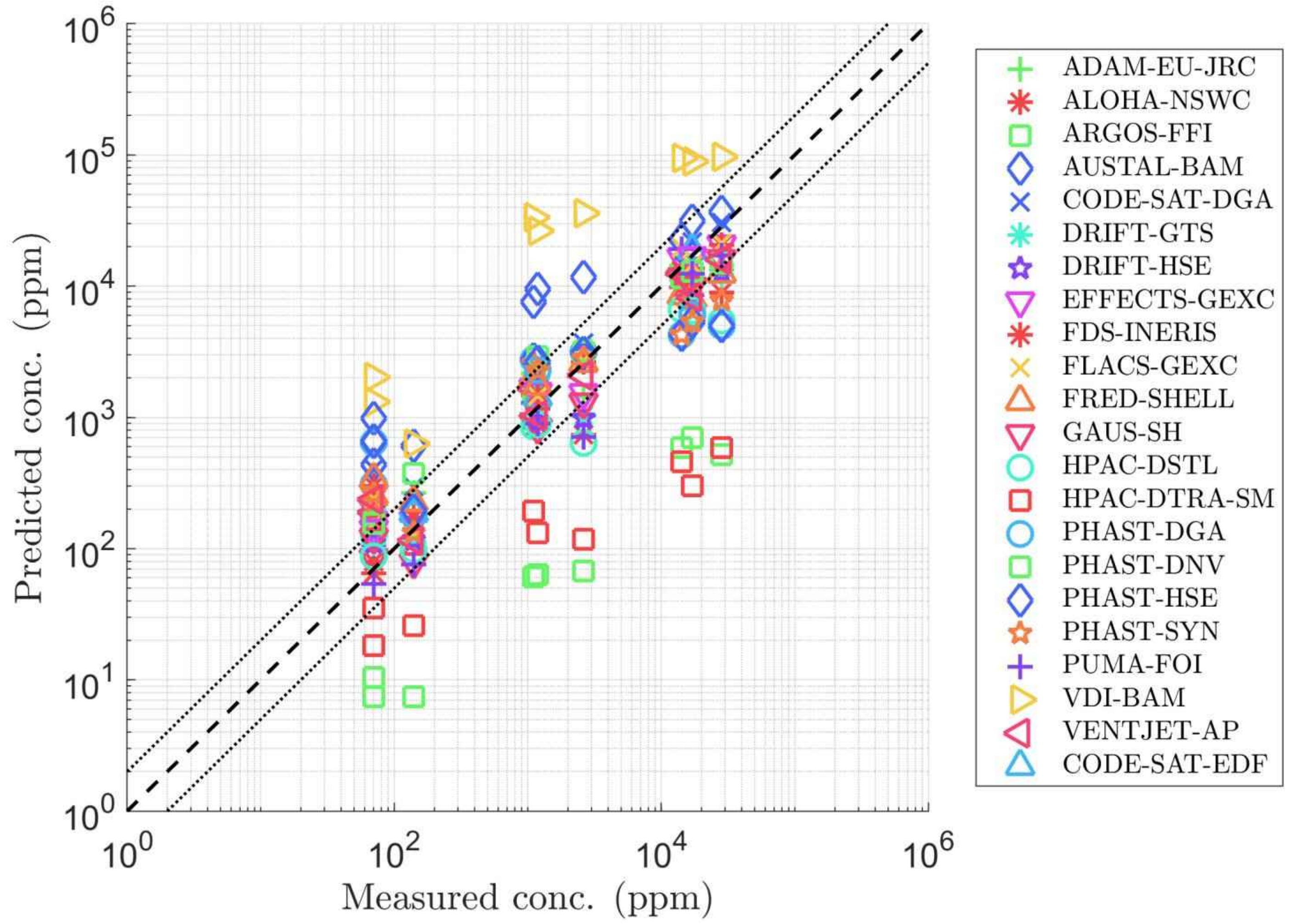
All results

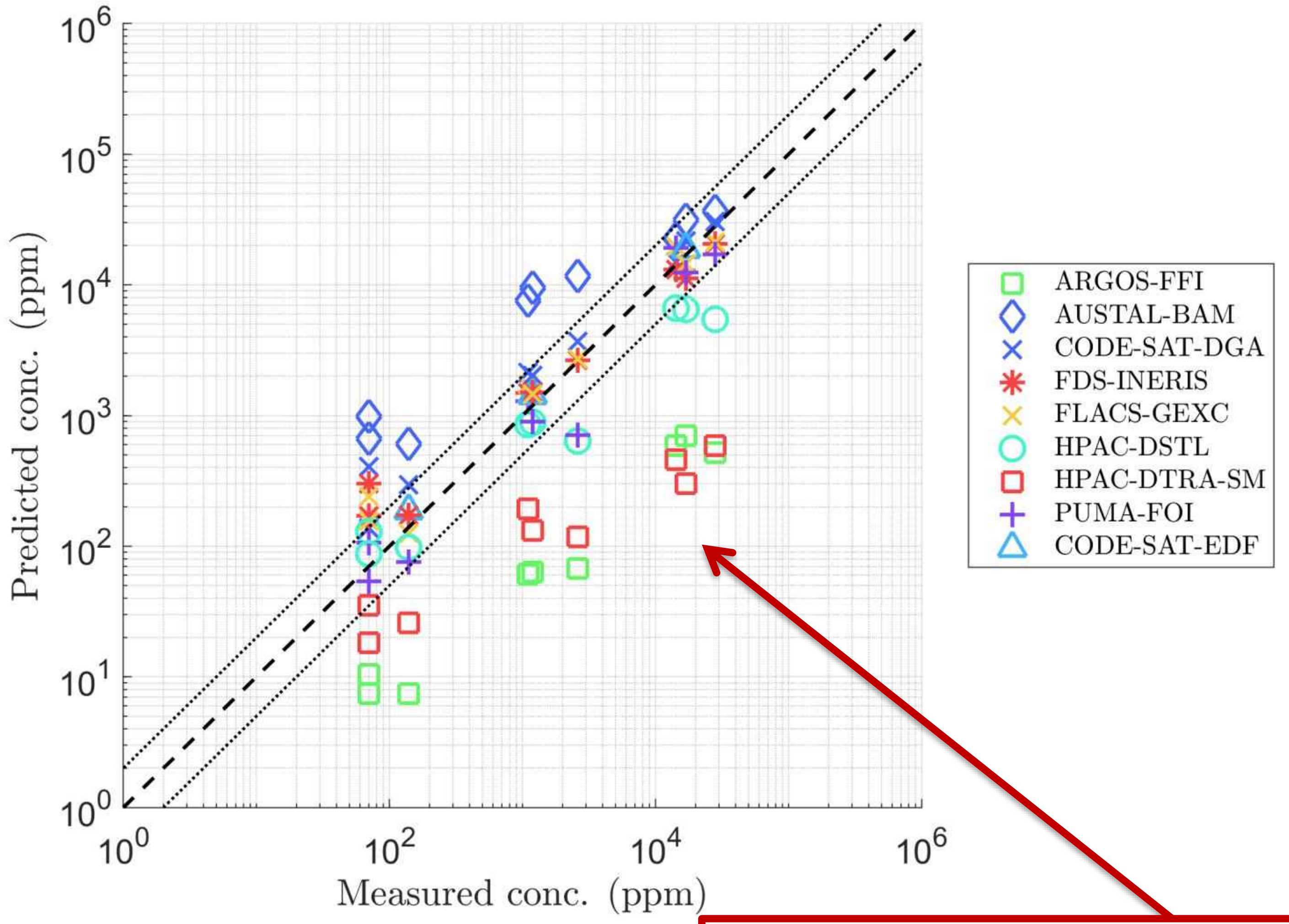
CFD, Gaussian puff, Lagrangian

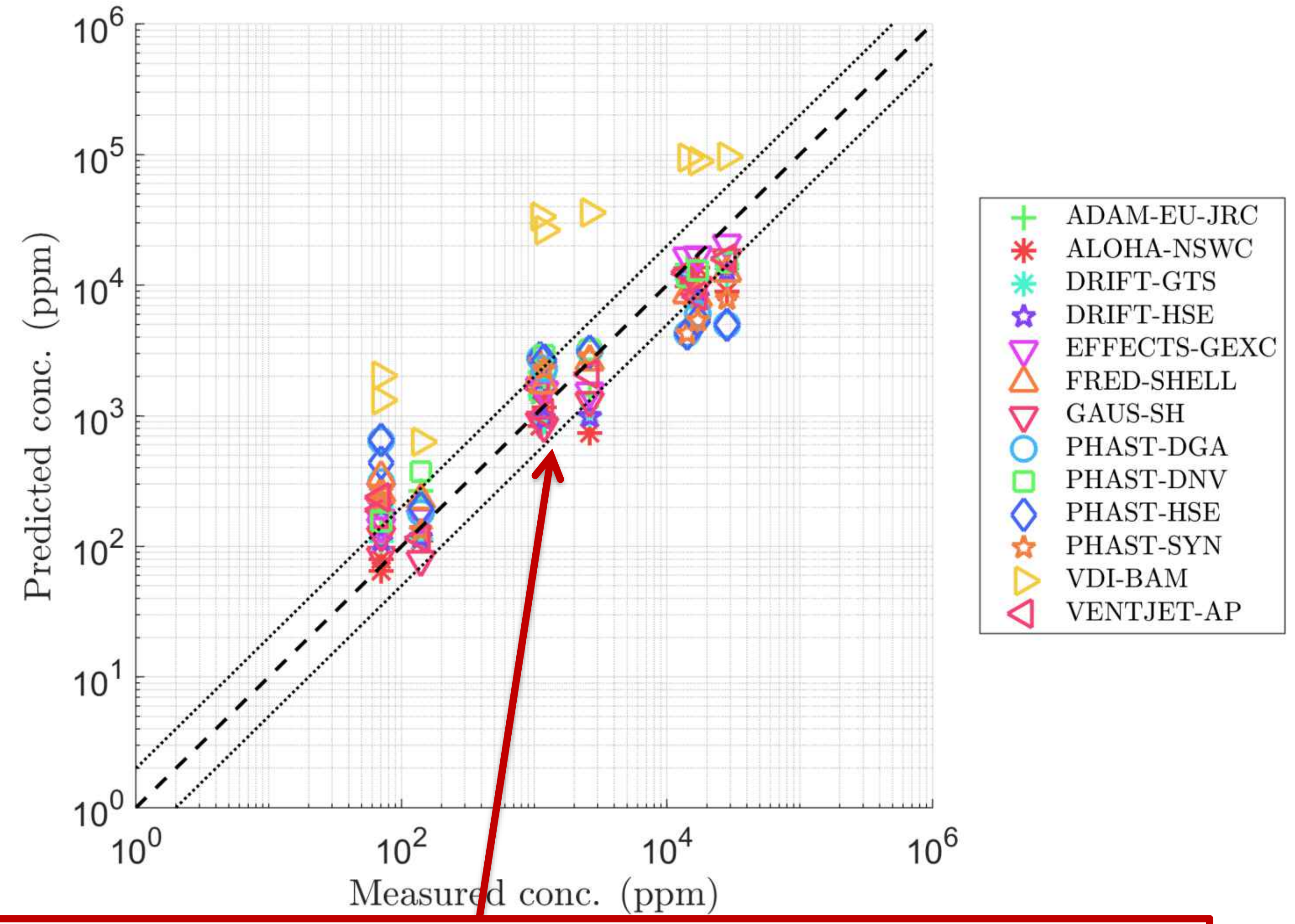
Empirically-based nomograms, integral, Gaussian plume

FLADIS

Predicted versus Measured Centerline Concentrations







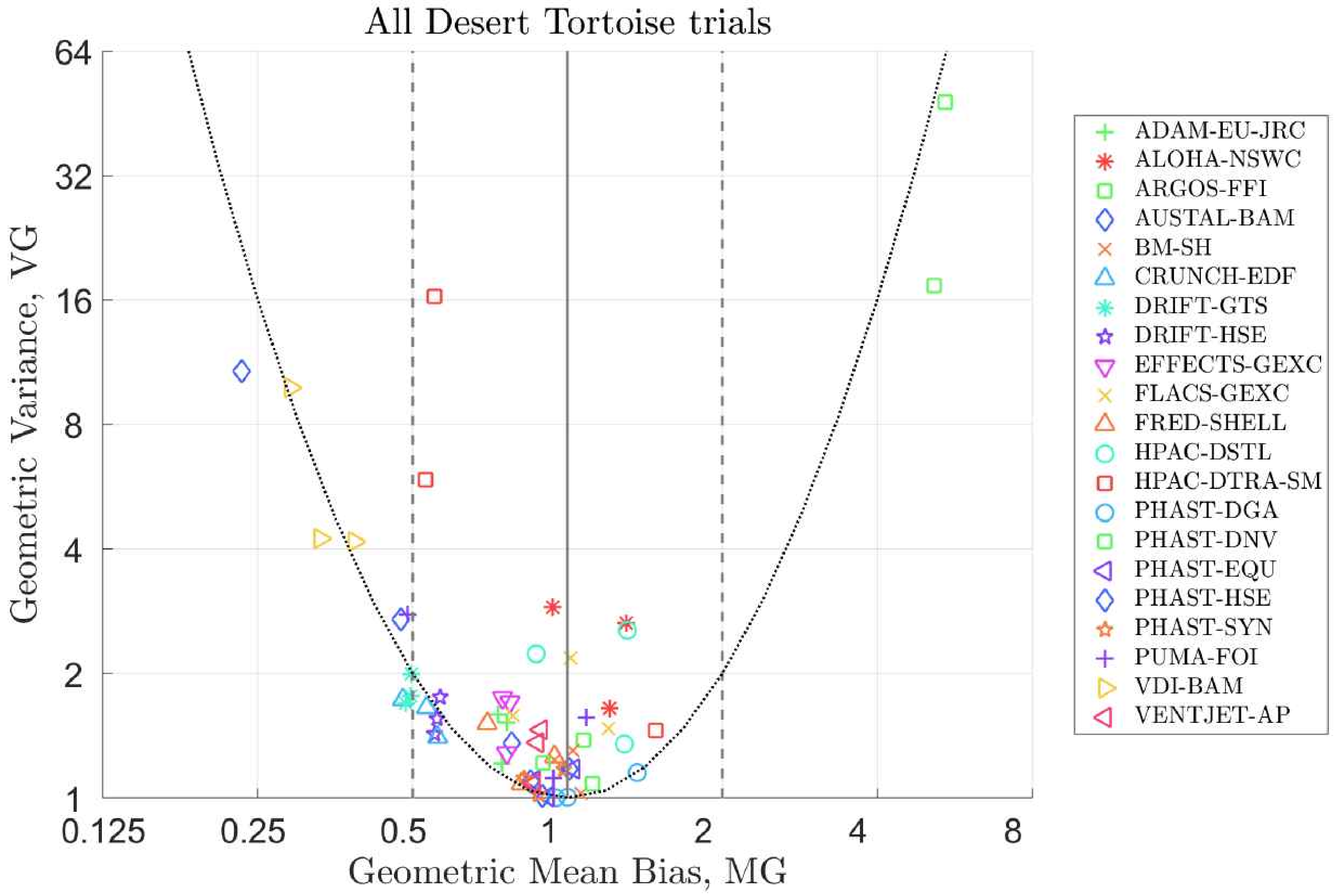
Generally less scatter with nomograms/integral/Gaussian plume models, with exception of VDI model

All results

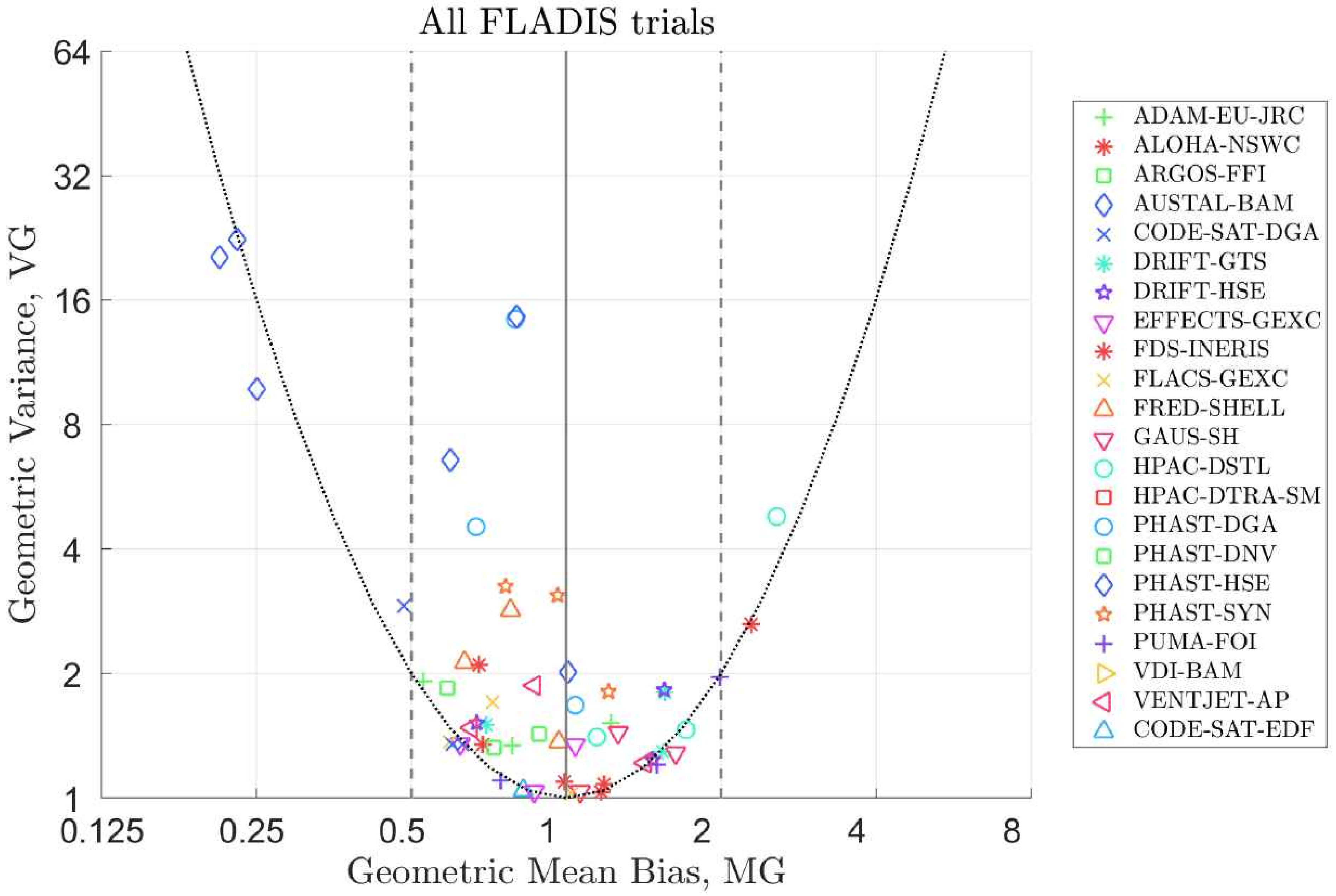
CFD, Gaussian puff, Lagrangian

Empirically-based nomograms, integral, Gaussian plume

Geometric Mean Bias versus Geometric Variance



Model over-predicts   Model under-predicts



Model over-predicts   Model under-predicts

$$MG = exp\left\langle \ln\left(\frac{C_m}{C_p}\right) \right\rangle \qquad VG = exp\left\langle \left[\ln\left(\frac{C_m}{C_p}\right)\right]^2 \right\rangle$$

Summary / Conclusions

- Strong USA/UK/European support for this initial JRIII modeling exercise
  - Total of 26 sets of model predictions provided by 21 independent groups
- Agreement between model predictions and measurements varied between different models
- Useful insights gained through discussions between participants into choice of modeling approach, including discussions between different groups all using the same model
  - Experience useful for some groups in improving modeling approach going forward for JRIII
- Sensitivity tests: relatively strong impact from vapor-only source specification
  - Can we take measurements in JRIII trials to reduce this uncertainty to modeling of source conditions?
  - Further work to follow on sensitivity analysis by DSTL (including ensemble modeling)
- Modeling exercise and analysis of the Desert Tortoise and FLADIS data provided useful insights into design of the future JRIII trials, e.g.:
  - Desert Tortoise trials highlighted the need for measurements to extend further downwind to capture dense-gas/passive/buoyant(?) dispersion, i.e., full extent of hazardous cloud
  - FLADIS trials also showed that releases of this scale do not exhibit significant dense-gas effects
- Future collaborative JRIII exercise could involve modeling a previous large-scale ammonia incident

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Acknowledgements

Many thanks to all modeling groups for their valuable contributions for this exercise

Thank you

Simon Gant[1], Joseph Chang[2], Sun McMasters[3], Ray Jablonski[3], Helen Mearns[3], Shannon Fox[3], Ron Meris[4], Scott Bradley[4], Sean Miner[4], Matthew King[4], Steven Hanna[5], Thomas Mazzola[6], Tom Spicer[7], Rory Hetherington[1], Alison McGillivray[1], Adrian Kelsey[1], Harvey Tucker[1], Graham Tickle[8], Oscar Björnham[9], Bertrand Carissimo[10], Luciano Fabbri[11], Maureen Wood[11], Karim Habib[12], Mike Harper[13], Frank Hart[13], Thomas Vik[14], Anders Helgeland[14], Joel Howard[15], Veronica Bowman[15], Daniel Silk[15], Lorenzo Mauri[16], Shona Mackie[16], Andreas Mack[16], Jean-Marc Lacome[17], Stephen Puttick[18], Adeel Ibrahim[18], Derek Miller[19], Seshu Dharmavaram[19], Amy Shen[19], Alyssa Cunningham[20], Desiree Beverley[20], Matthew O'Neal[20], Laurent Verdier[21], Stéphane Burkhart[21], Chris Dixon[22], Sandra Nilsen[23]

[1]RAND Corporation,[2]Health and Safety Executive (HSE),[3]Chemical Security Analysis Center (CSAC), Department of Homeland Security (DHS), [4]Defense Threat Reduction Agency (DTRA), [5]Hanna Consultants, Inc., [6]Systems Planning and Analysis, Inc. (SPA), [7]University of Arkansas, [8]GT Science and Software, [9]Swedish Defence Research Agency (FOI), [10]EDF/Ecole des Ponts, [11]European Joint Research Centre (JRC), [12]Bundesanstalt für Materialforschung und -prüfung (BAM), [13]DNV, Stockport, [14]Norwegian Defence Research Establishment (FFI), [15]Defence Science and Technology Laboratory (DSTL), [16]Gexcon, [17]Institut National de l'Environnement Industriel et des Risques (INERIS), [18]Syngenta, [19]Air Products, [20]Naval Surface Warfare Center (NSWC), [21]Direction Générale de l'Armement (DGA), [22]Shell, [23]Equinor

Contact points:
Joe Chang (jchang@rand.org)
Simon Gant (simon.gant@hse.gov.uk)

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Predicted vs Measured Centerline Concentrations

RESEARCH AND GUIDANCE FROM HSE

Baseline Model	DT1		DT2		DT4		FLADIS9			FLADIS16			FLADIS24		
	100m	800m	100m	800m	100m	800m	20m	70m	238m	20m	70m	238m	20m	70m	238m
ADAM-EU-JRC	117112	6384	154475	10553	143547	12351	14411	2157	238	10990	1996	267	14404	1437	137
ALOHA-NSWC	98384	2609	136035	4569	171313	6370	9841	837	80	13690	1165	111	8974	740	65
ARGOS-FFI	11447	569	23940	1417	28937	1123	587	61	7	702	63	7	517	68	10
AUSTAL-BAM	104000	6886	586000	28600	234000	18100	22600	7600	667	31300	9470	608	36800	11700	988
CODE-SAT-DGA	-	-	-	-	-	-	14989	2125	138	21800	2034	294	30558	3691	405
CODE-SAT-EDF	-	-	-	-	-	-	-	-	-	18765	1433	188	-	-	-
BM-SH	82865	5877	90638	8859	93336	9749	-	-	-	-	-	-	-	-	-
CRUNCH-EDF	107680	17672	112747	28378	100798	30313	-	-	-	-	-	-	-	-	-
DRIFT-GTS	155947	11319	174294	22120	152100	25615	11187	1443	199	7579	894	115	12195	1028	109
DRIFT-HSE	142405	9534	156941	18926	141061	21770	11912	1508	202	8104	938	117	12689	983	111
EFFECTS-GEXC	126894	5746	165882	9398	152307	11193	16658	1680	162	16868	1566	165	20835	1530	143
FDS-INERIS	-	-	-	-	-	-	13144	1486	171	11207	1506	172	20700	2650	301
FLACS-GEXC	118013	3584	125254	5011	137370	11323	19499	1722	155	14470	1453	126	21359	2695	240
GAUS-SH							11668	915	85	9895	833	79	16169	1305	122
HPAC-DSTL	95614	2657	104598	5186	159609	7915	6622	851	129	6498	890	98	5463	642	87
HPAC-DTRA-SM	53559	3700	504253	6399	495409	6358	458	194	35	300	132	26	590	118	18
PHAST-DGA	46096	9419	85734	11740	51786	9898	4256	2766	311	6069	2287	180	4967	3158	648
PHAST-DNV	80899	4654	96505	7501	98310	12113	11592	1541	161	12916	2917	372	14947	3186	155
PHAST-HSE	75588	8007	91726	12332	85144	11056	4268	2765	437	5327	2652	196	4959	3108	653
PHAST-SYN	78982	8117	90870	12853	86736	11374	4266	2556	227	5324	2281	132	4962	2728	256
PUMA-FOI	88366	4147	122102	8386	239535	16667	19252	1290	106	12378	898	76	17121	707	54
VDI-BAM	264000	11100	400000	20700	470000	24200	94800	33300	1309	88900	26500	629	96700	36000	2030
VENTJET-AP	96962	5865	122778	9952	118191	10257	12476	1657	189	8224	1030	116	15918	2092	238
Experiment	**49490**	**8790**	**82920**	**10910**	**57300**	**16678**	**14190**	**1100**	**70**	**17010**	**1190**	**140**	**28180**	**2610**	**70**

Sensitivity Tests

- Aim: to understand potential impact of experimental uncertainties and modeling options
- Suggestions given in model exercise specification documents:

1.) Standing water at the Frenchman Flats test site in Desert Tortoise trials DT1 and DT2

		DT1	DT2
Relative humidity (%)	Baseline	13.2	17.5
	Sensitivity test	50	50
Monin-Obukhov length (m)	Baseline	92.7	94.7
	Sensitivity test	-20	-20
Pasquill stability class	Baseline	D	D
	Sensitivity test	C	C

2.) Wind speed variability in DT4

		DT4
Site average wind speed (m/s)	Baseline	4.51
	Sensitivity test	3.0

3.) Ammonia liquid rainout in the Desert Tortoise trials

- For models that have the capability to simulate a fixed fraction of liquid raining out from the jet and depositing to form an evaporating pool on the ground:

		DT1	DT2	DT4
Rainout mass fraction (%)	Baseline	5	5	5
	Sensitivity test (min)	0	0	0
	Sensitivity test (max)	20	36	30

- Tests could also be performed with rainout sub-models (if available)
- Compare predicted size of deposited ammonia pool to observed wetted area, if possible

4.) Pasquill Stability Classes in DT4, FLADIS16 and FLADIS24

- For models that use Pasquill stability class instead of Monin-Obukhov length to specify the model atmospheric boundary layer, the following tests could be undertaken:

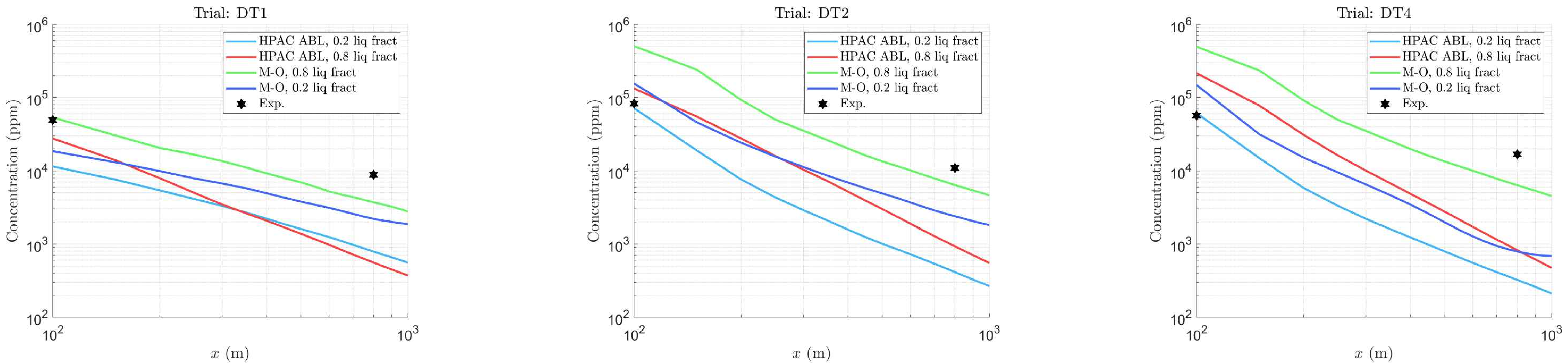
		DT4	FLADIS16	FLADIS24
Pasquill stability class	Baseline	D	D	C
	Sensitivity test	E	E	D

5.) Wind and turbulence profiles in the FLADIS trials

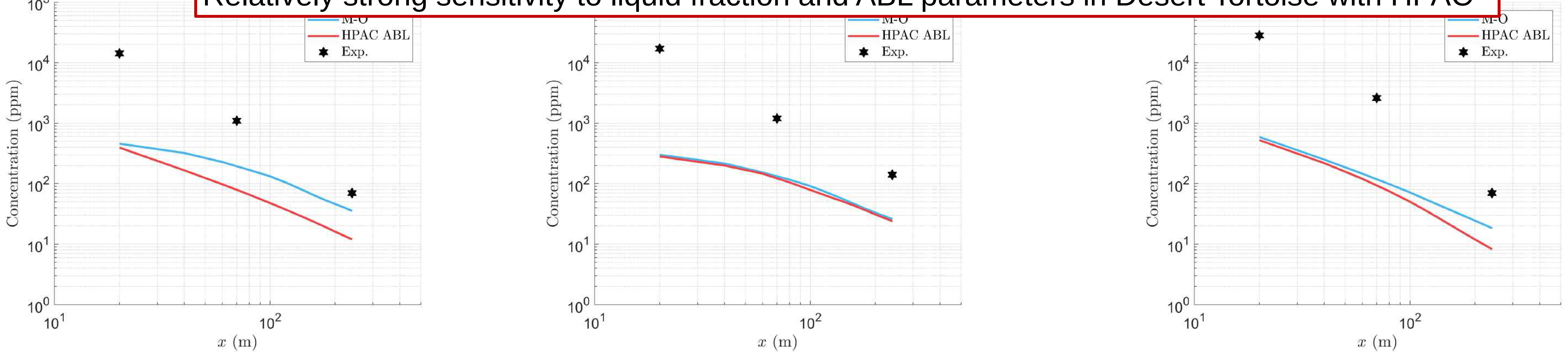
- Use wind profiles specified in the SMEDIS database and turbulence conditions specified in Table 8 or those extracted directly from the FLADIS dataset measurements (if possible).

Some modelers have examined additional factors, e.g., specification of equivalent vapor-only source conditions

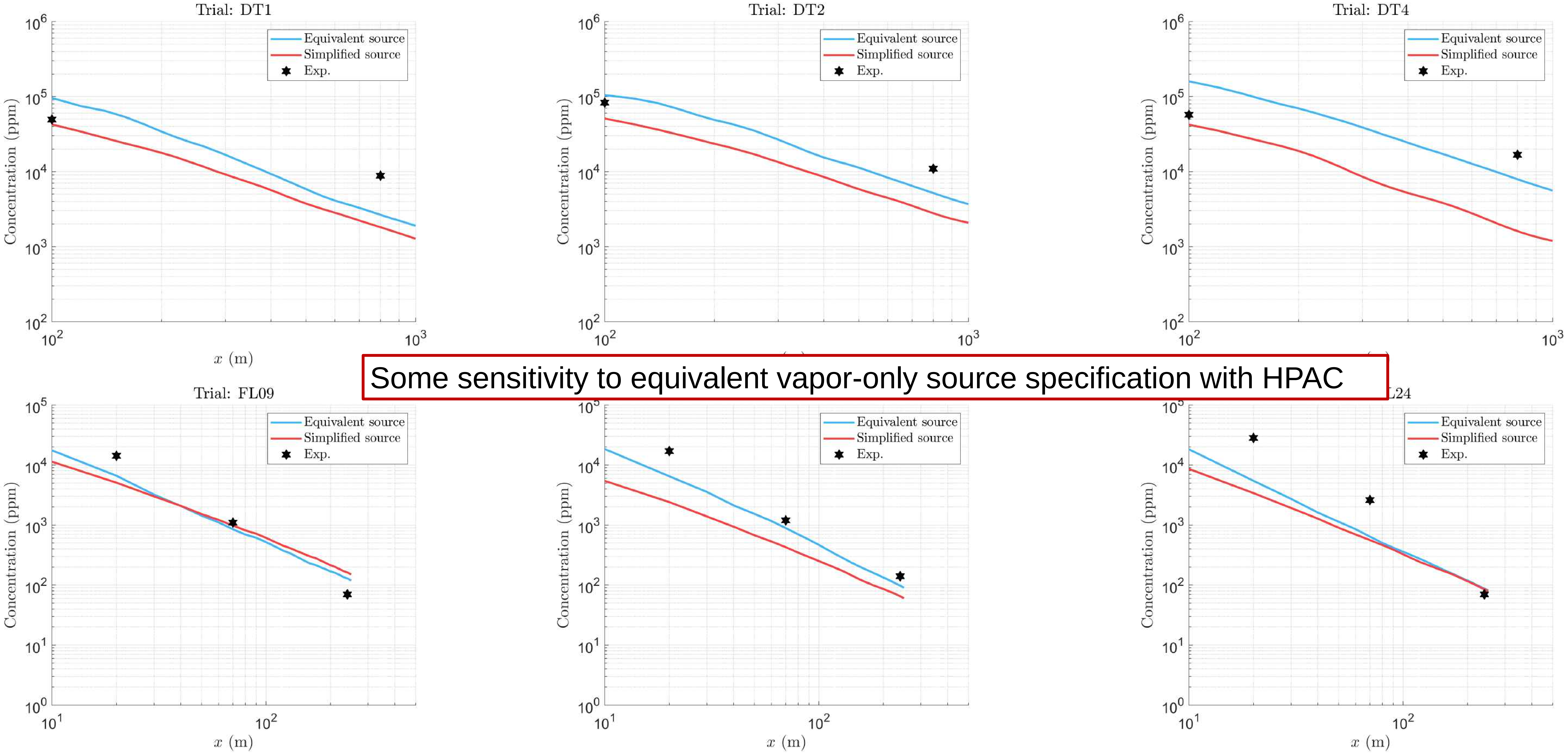
Sensitivity Tests: DTRA Albuquerque (Sean Miner)



Relatively strong sensitivity to liquid fraction and ABL parameters in Desert Tortoise with HPAC

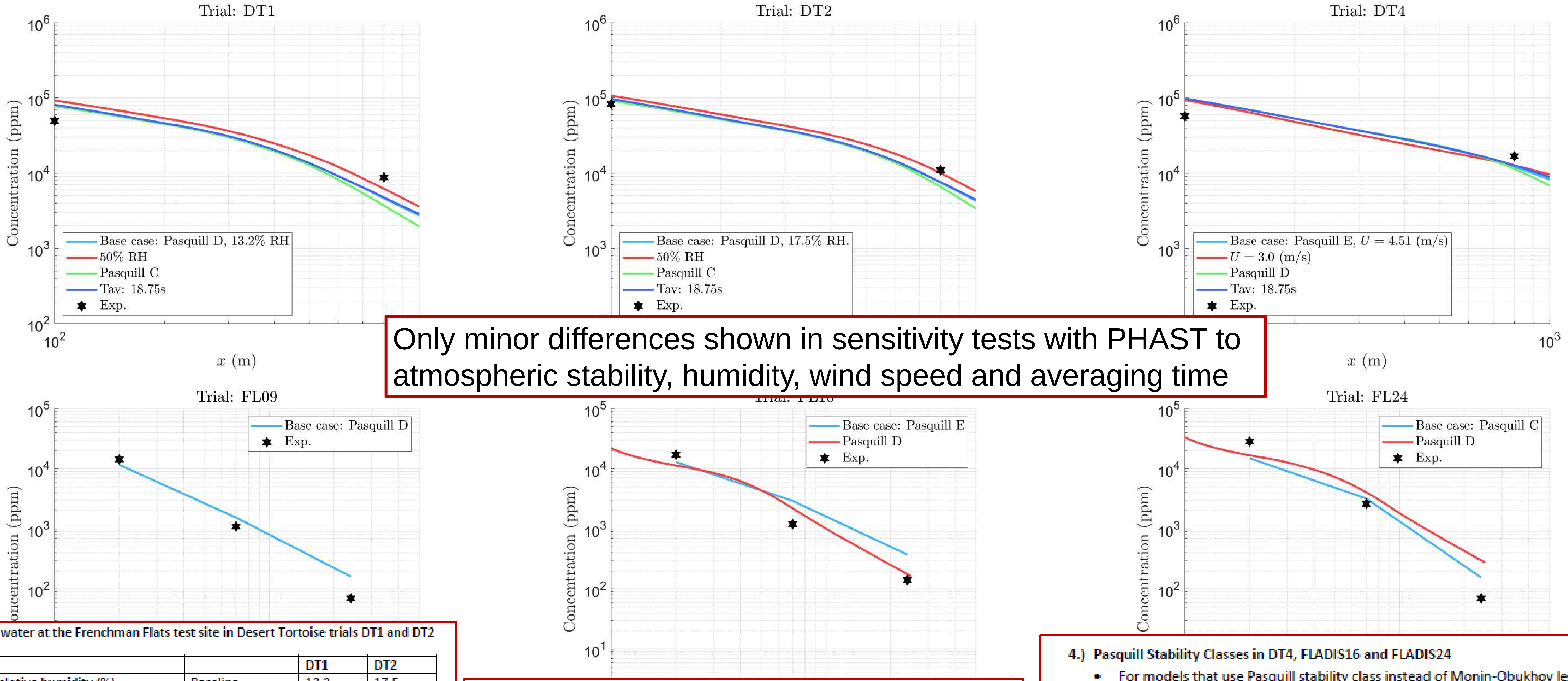


Sensitivity Tests: Dstl (Joel Howard)



Some sensitivity to equivalent vapor-only source specification with HPAC

Sensitivity Tests: PHAST (Frank Hart)



Only minor differences shown in sensitivity tests with PHAST to atmospheric stability, humidity, wind speed and averaging time

1.) Standing water at the Frenchman Flats test site in Desert Tortoise trials DT1 and DT2

		DT1	DT2
Relative humidity (%)	Baseline	13.2	17.5
	Sensitivity test	50	50
Monin-Obukhov length (m)	Baseline	92.7	94.7
	Sensitivity test	-20	-20
Pasquill stability class	Baseline	D	D
	Sensitivity test	C	C

2.) Wind speed variability in DT4

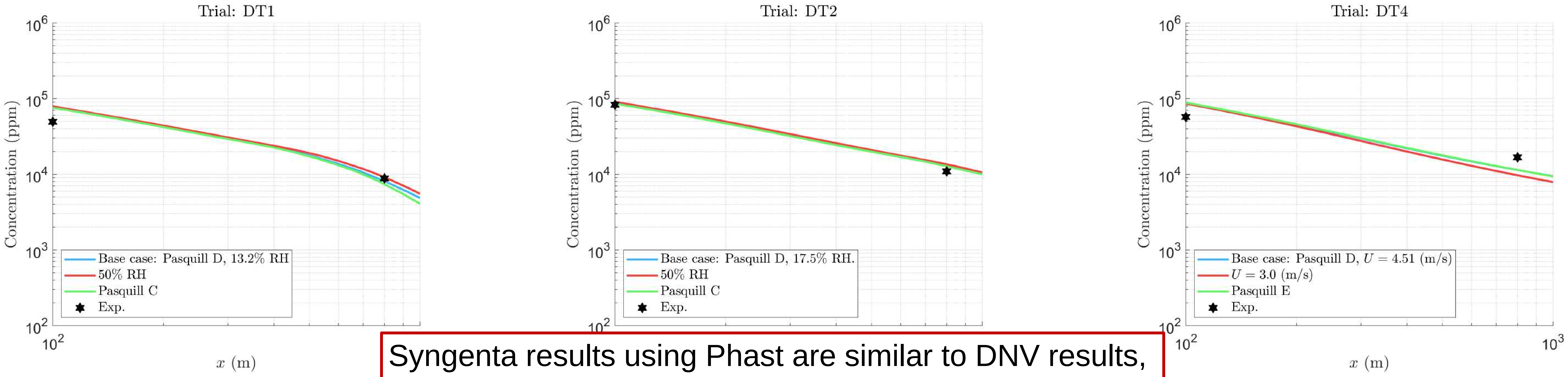
		DT4
Site average wind speed (m/s)	Baseline	4.51
	Sensitivity test	3.0

4.) Pasquill Stability Classes in DT4, FLADIS16 and FLADIS24

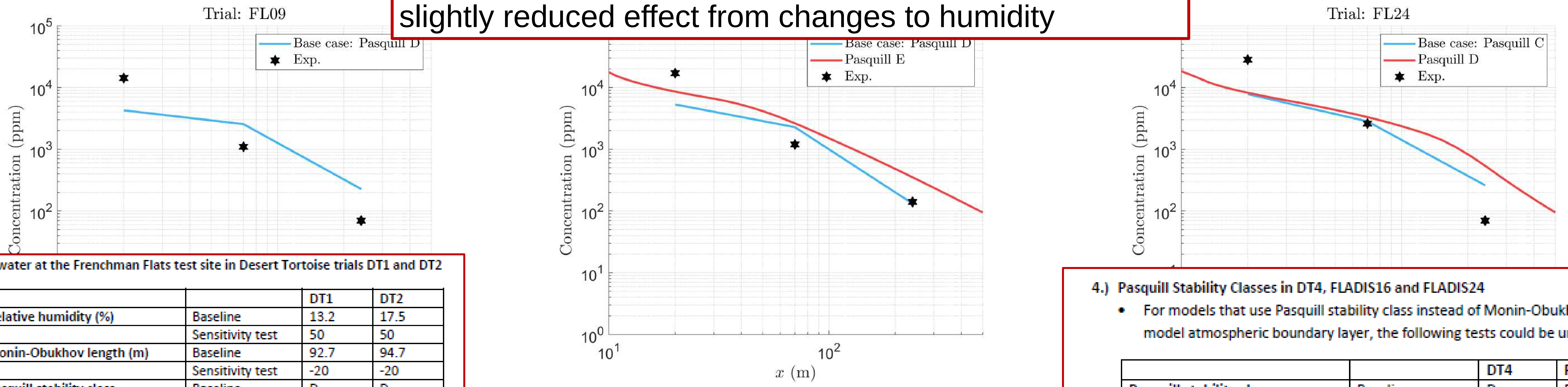
- For models that use Pasquill stability class instead of Monin-Obukhov length to specify the model atmospheric boundary layer, the following tests could be undertaken:

		DT4	FLADIS16	FLADIS24
Pasquill stability class	Baseline	D	D	C
	Sensitivity test	E	E	D

Sensitivity Tests: PHAST-SYN (Adeel Ibrahim)



Syngenta results using Phast are similar to DNV results, slightly reduced effect from changes to humidity



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		DT1	DT2
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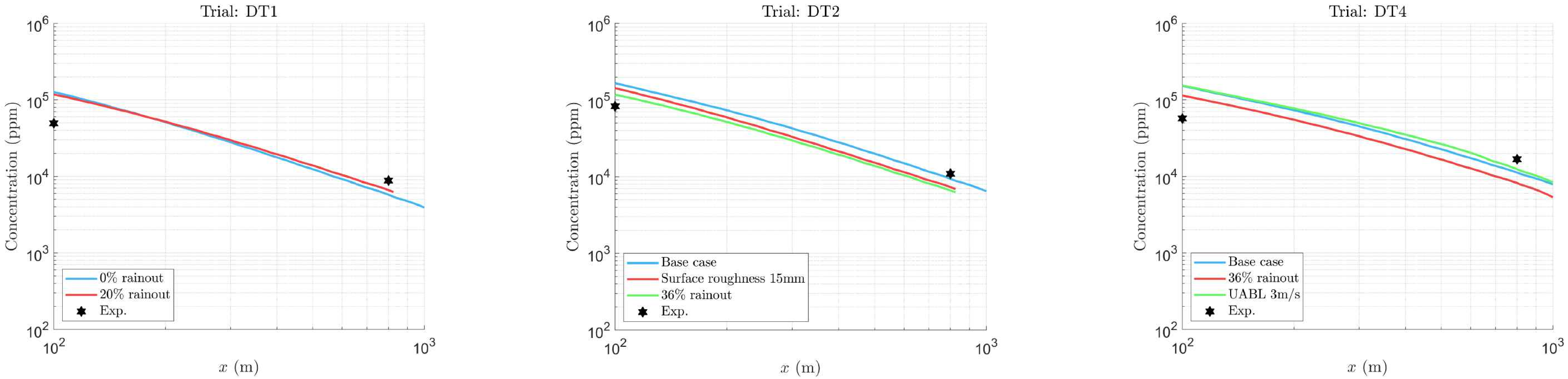
Pasquill stability class	Baseline	D	D
	Sensitivity test	C	C

4.) Pasquill Stability Classes in DT4, FLADIS16 and FLADIS24

- For models that use Pasquill stability class instead of Monin-Obukhov length to specify the model atmospheric boundary layer, the following tests could be undertaken:

		DT4	FLADIS16	FLADIS24
Pasquill stability class	Baseline	D	D	C
	Sensitivity test	E	E	D

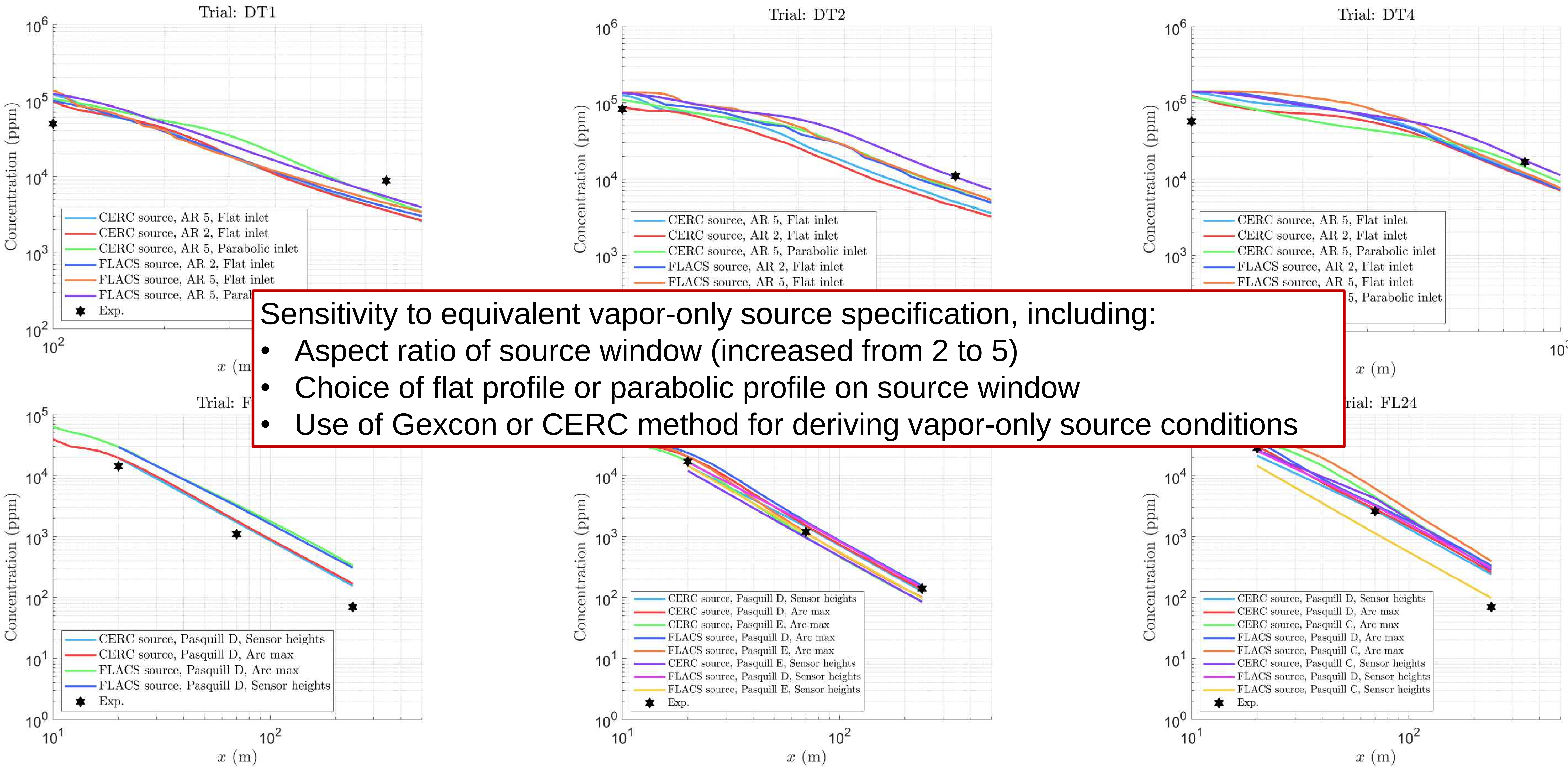
Sensitivity Tests: EFFECTS-GEXC (Andreas Mack)



Minor sensitivity to:

- Increased liquid rainout from 0% to 20% or 36%
- Surface roughness increased from 3 mm (base case) to 15 mm
- Wind speed reduced from 4.5 m/s to 3.0 m/s in DT4

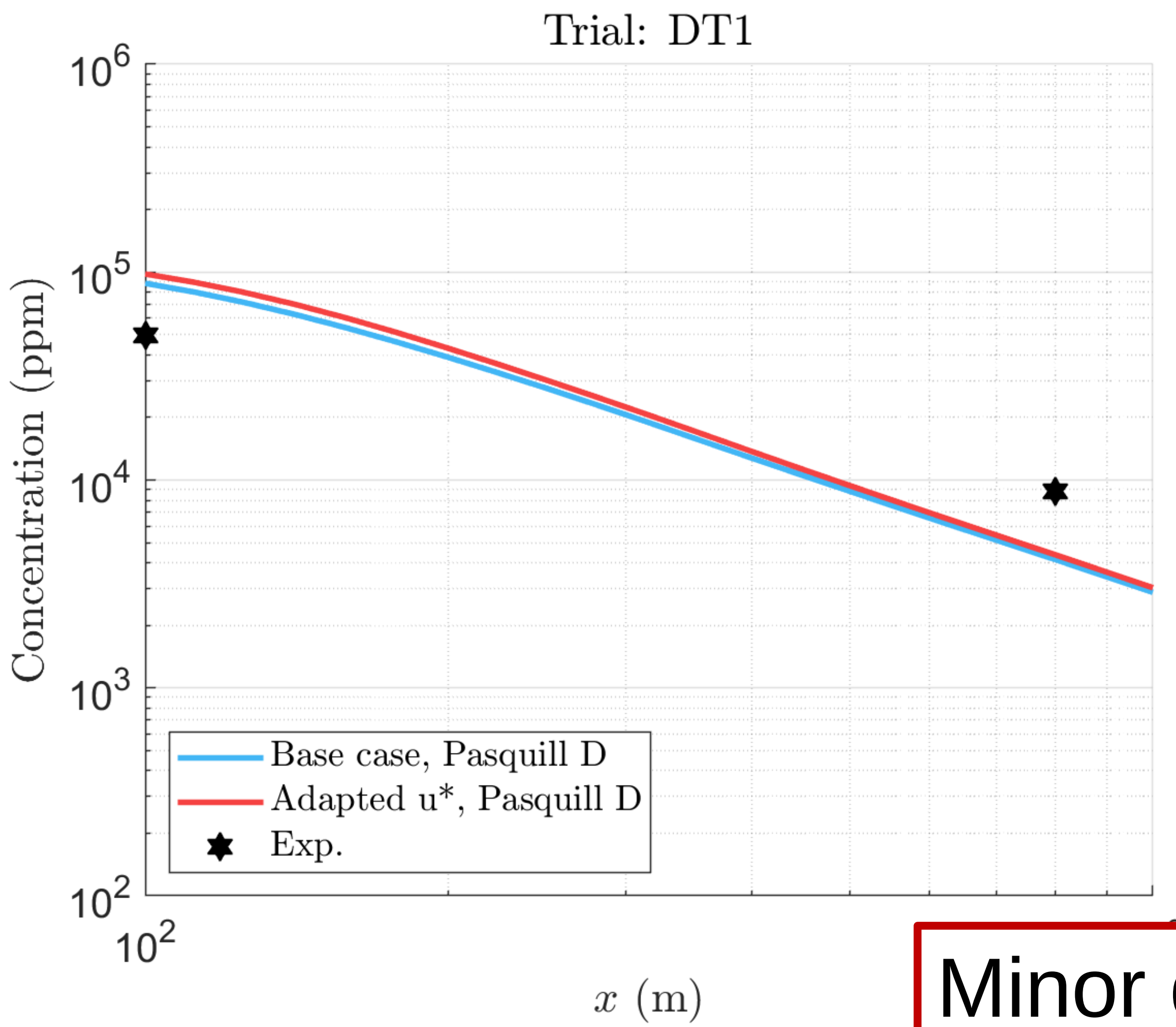
Sensitivity Tests: FLACS-GEXC (Lorenzo Mauri)

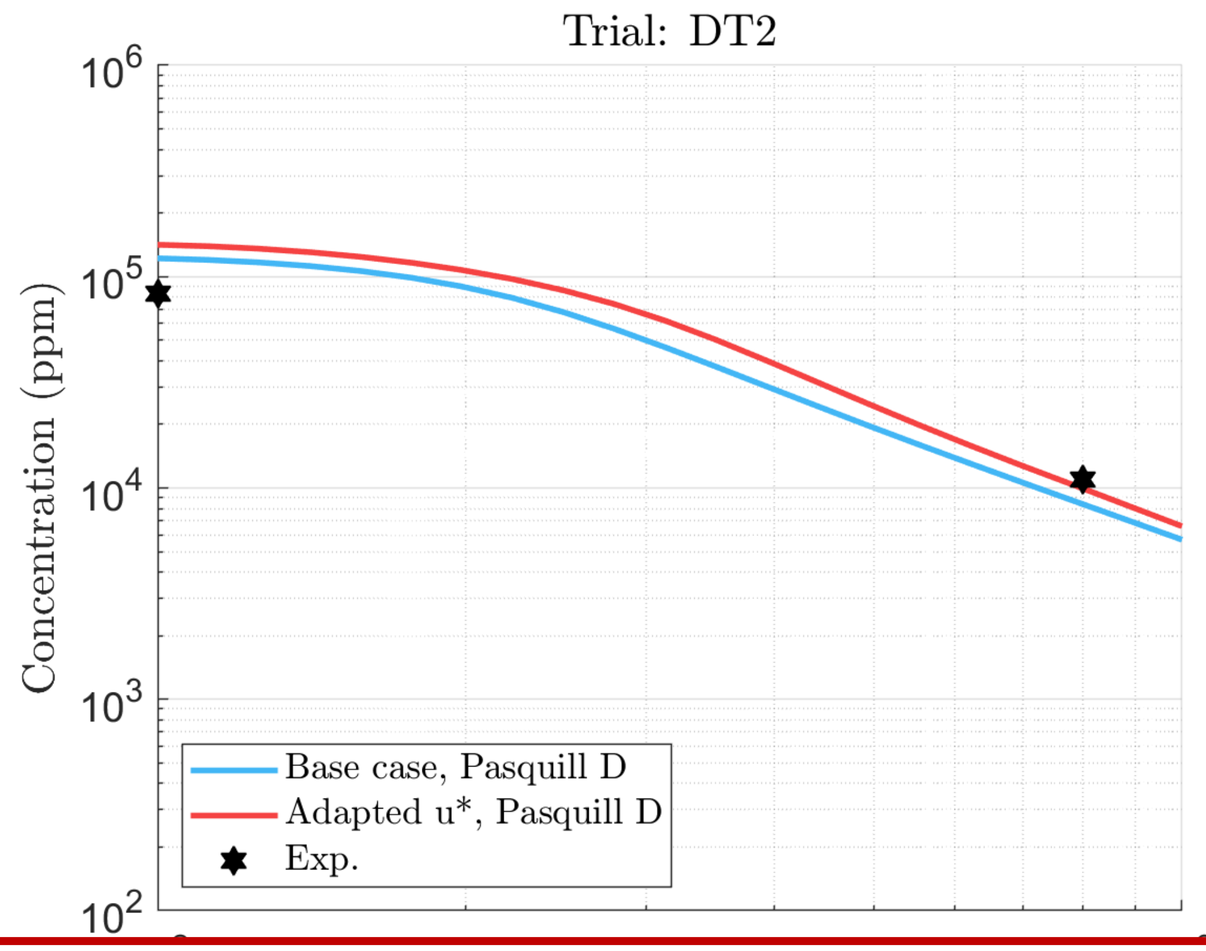


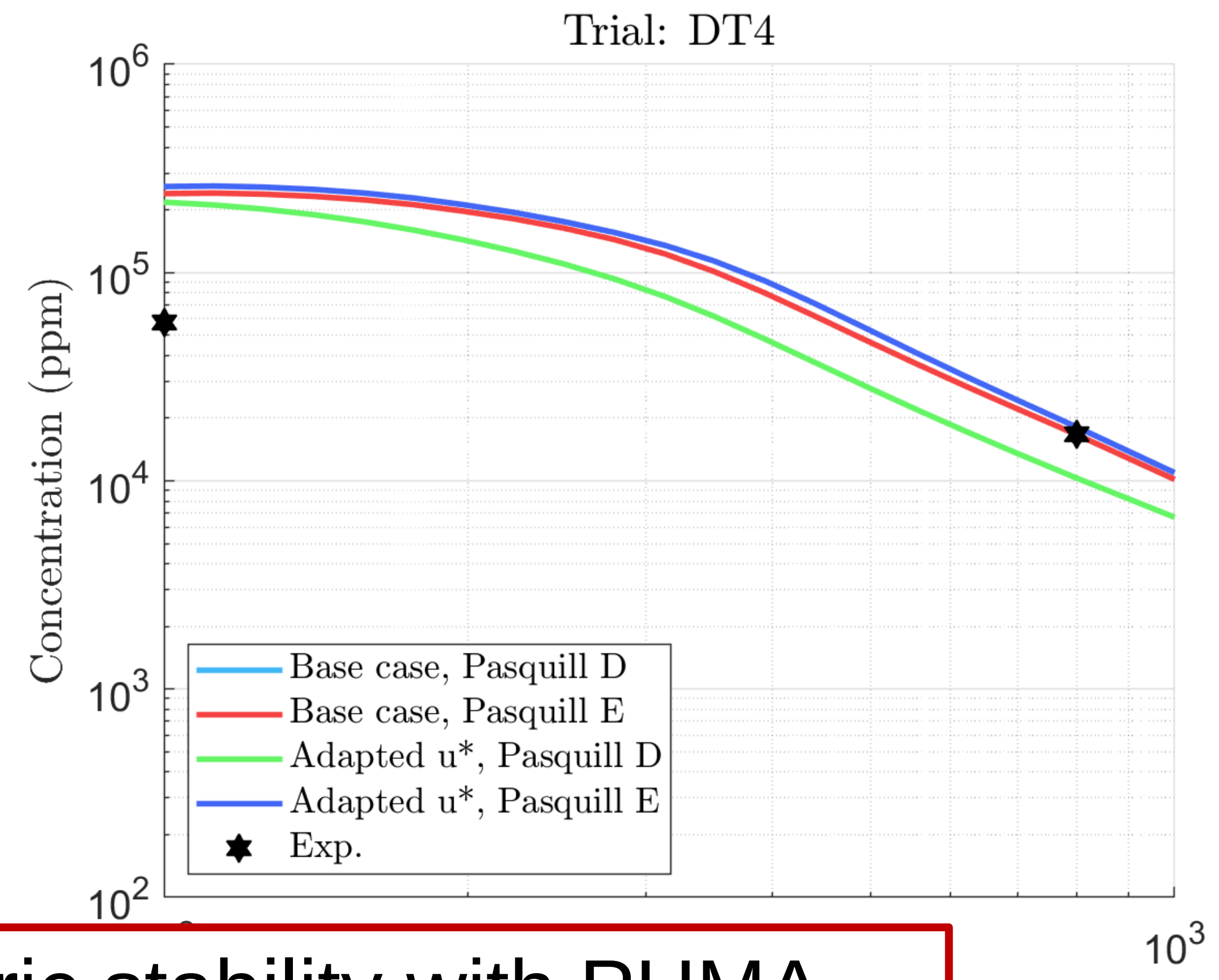
Sensitivity to equivalent vapor-only source specification, including:

- Aspect ratio of source window (increased from 2 to 5)
- Choice of flat profile or parabolic profile on source window
- Use of Gexcon or CERC method for deriving vapor-only source conditions

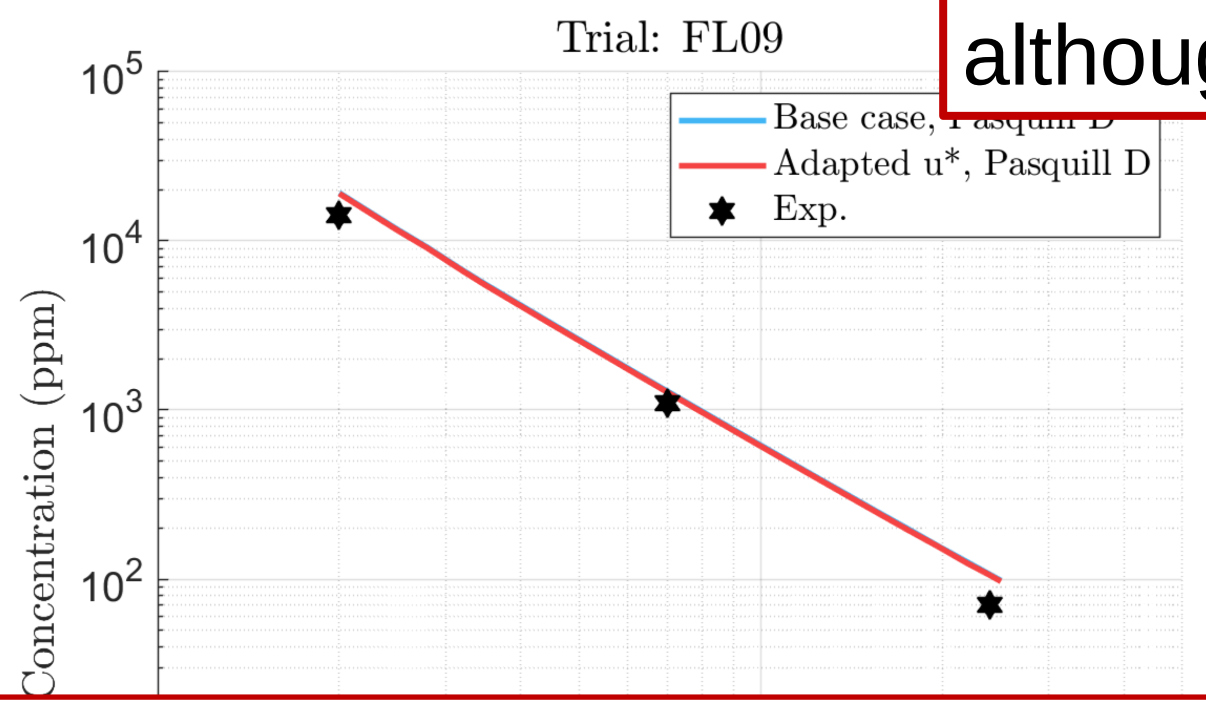
Sensitivity Tests: PUMA-FOI (Oscar Björnham)

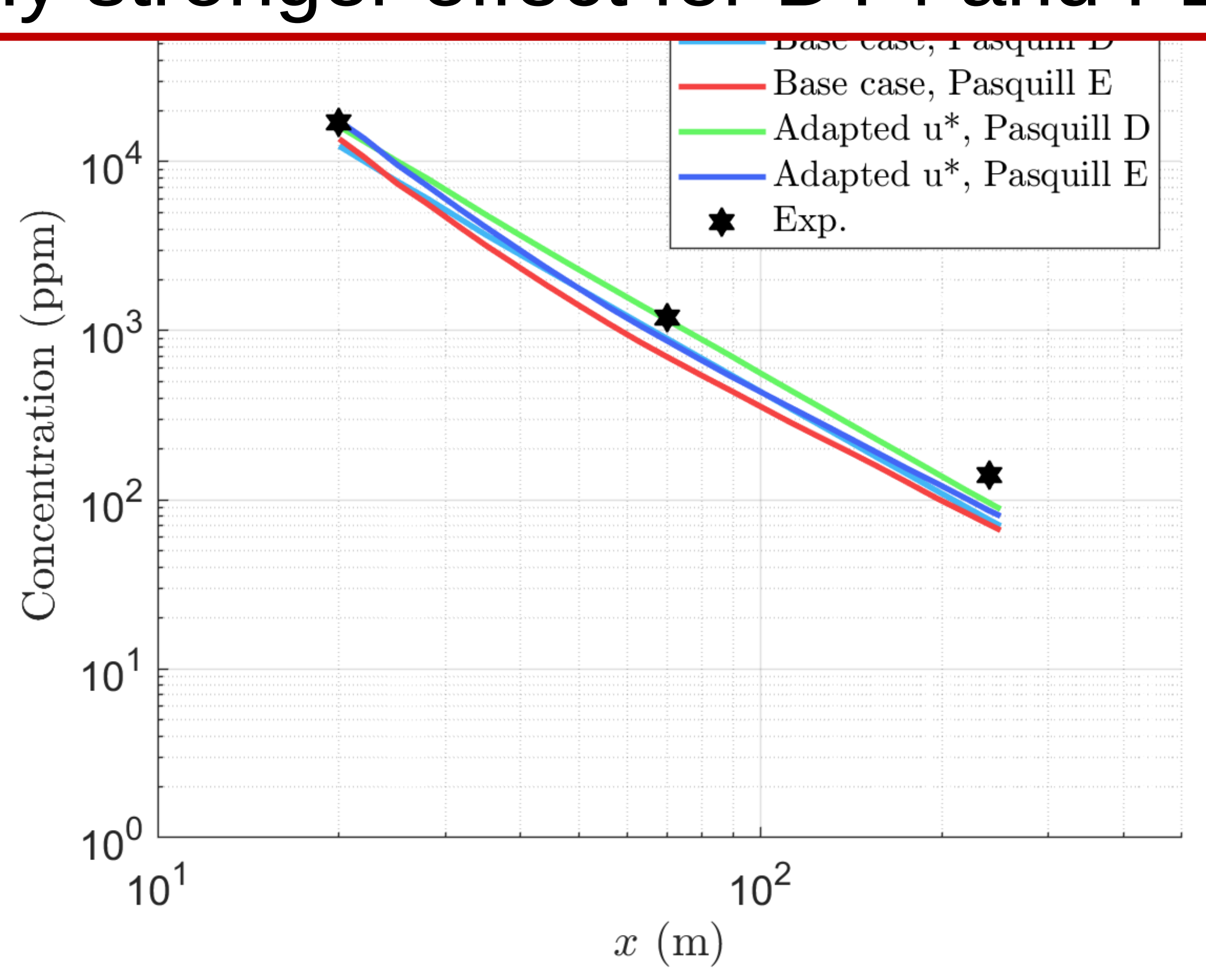


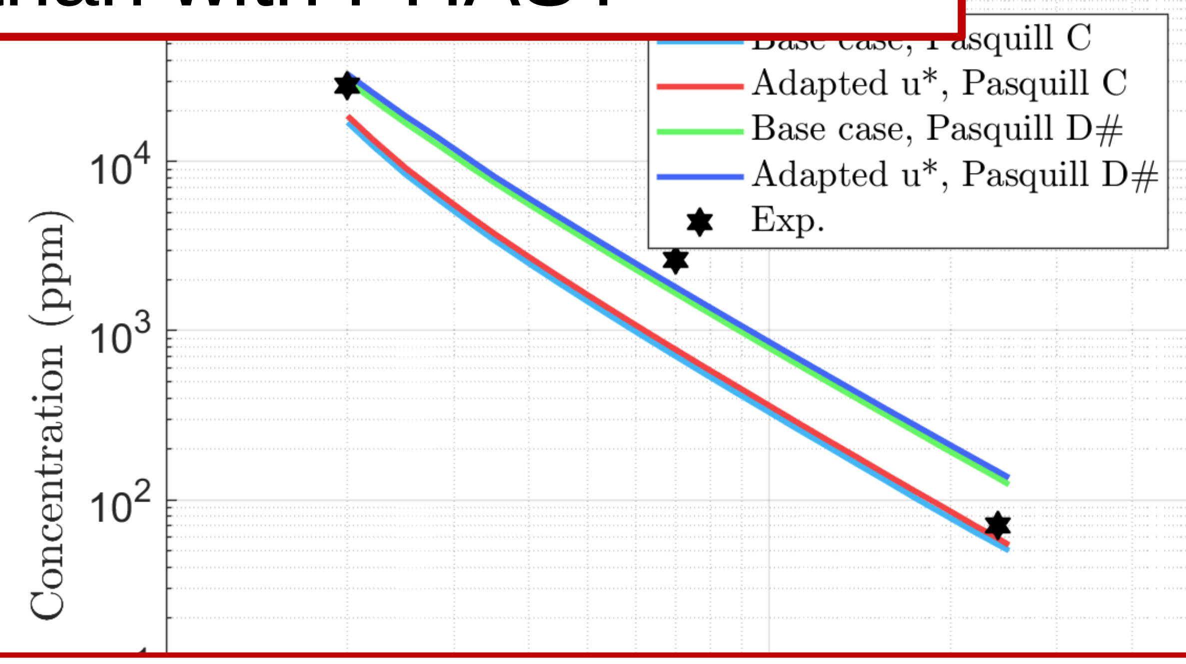




Minor differences shown in sensitivity tests to atmospheric stability with PUMA, although slightly stronger effect for DT4 and FLADIS24 than with PHAST







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Pasquill stability class	Baseline	D	D
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4.) Pasquill Stability Classes in DT4, FLADIS16 and FLADIS24

- For models that use Pasquill stability class instead of Monin-Obukhov length to specify the model atmospheric boundary layer, the following tests could be undertaken:

		DT4	FLADIS16	FLADIS24
Pasquill stability class	Baseline	D	D	C
	Sensitivity test	E	E	D