

Jack Rabbit III Modelers Working Group: Initial Model Inter-comparison Exercise for 2021-22

INERIS contribution

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Meteorological flow and dispersion with Fire Dynamic Simulator (FDS) (V6.7 - NIST Special Publication 1019 Sixth Edition Fire Dynamics Simulator User's Guide)

Modeling of FLADIS Trials

Set up of FDS

- / Domain – Mesh
- / Meteorological input
- / Source term

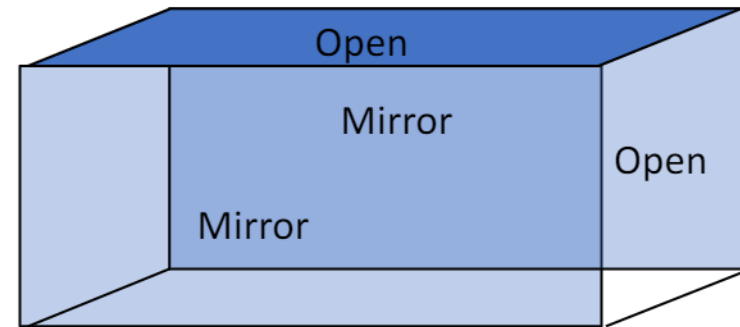
Main results

Meteorological flow and dispersion : which approach ?

Approach : Large Eddy Simulation

Precursor flow : Synthetic Eddy method (SEM) (Jarrin et al., 2006)

Precursor flow and dispersion domain



Ground surface : wall function (WALE)

SEM and meteorological input process :

Initial Modeling Exercise (2021-2022) : u_{10} , u^* , velocity fluctuation, Monin length and roughness



FDS Input : Wind Profile, rms , eddy length scale

Set up of FDS

Domain :

- / 640 m x 256 m x 64 m

Mesh :

- / Divided in 120 blocs
- / Regular Mesh
- / Mesh refining : Cell size around release point : 0.25 m, 0.5 m, 1 m, 2 m

Source term : equivalent source conditions

- / See Initial Modeling Exercise (2021-2022) - Version 2.3, 21 December 2021. Joseph Chang and Simon Gant.

Meteorological input

- / See Initial Modeling Exercise (2021-2022) - Version 2.3, 21 December 2021. Joseph Chang and Simon Gant.
- / FLADIS Geometry and Wind Directions - Version 1.0, 7 December 2021. Joseph Chang and Simon Gant.

Source term : equivalent source conditions

Initial Modeling Exercise (2021-2022) - Version 2.3, 21 December 2021

FLADIS

Trial	Flash Fraction	Density (kg/m ³)	Temperature (K)	Diameter (m)	Velocity (m/s)
FLADIS9	0.16	5.69	239.7	0.04	65.17
FLADIS16	0.17	-	239.7	0.031	65.85
FLADIS24	0.17	-	239.7	0.045	55.87

Circular source window

1. Conditions at end of flashing phase

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Density (kg/m ³)	Temperature (K)	Diameter (m)
FLADIS9	4.2	4.75	12	1.67	203.7	0.88
FLADIS16	3.1	5.12	12	1.64	203.9	0.73
FLADIS24	4.4	4.22	12	1.64	204.0	1.06

2. Conditions at location where all the ammonia liquid has vaporized

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Emissive surface : 10 cells

Mesh Constraint → set up of a velocity release lower than real velocity to respect the mass flow rate

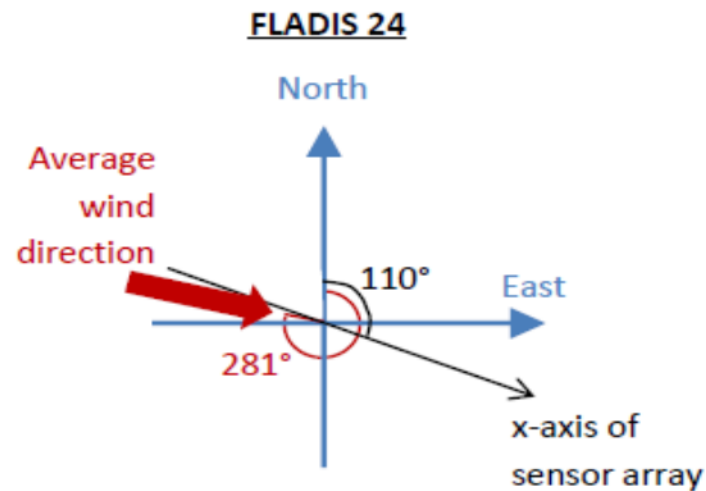
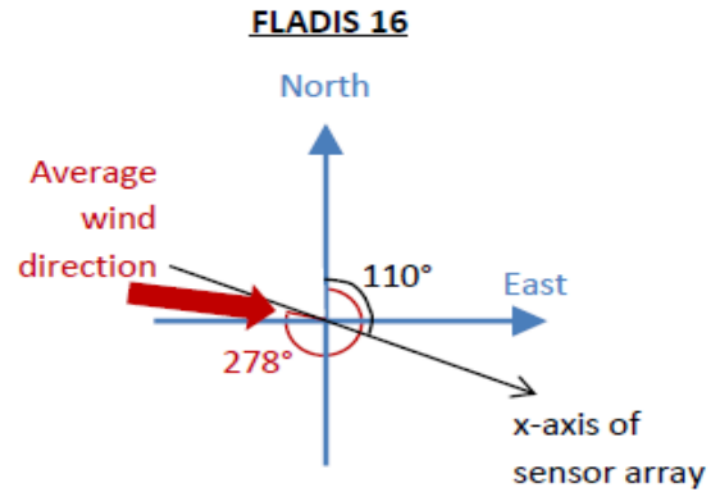
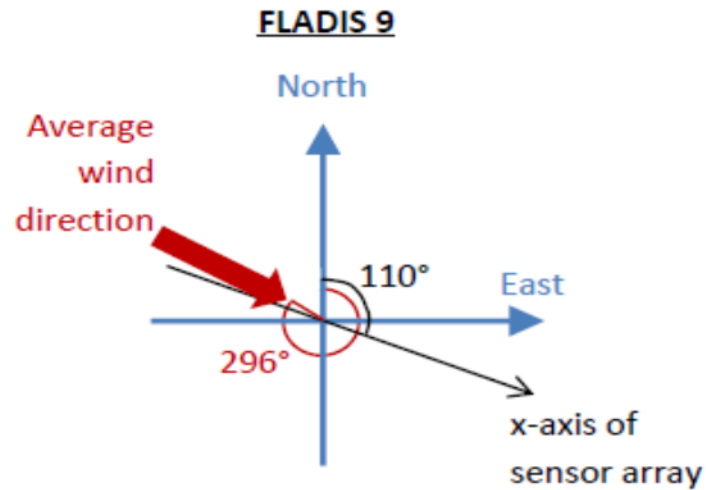
Meteorological input

Initial Modeling Exercise (2021-2022) - Version 2.3, 21 December 2021

		FLADIS9	FLADIS16	FLADIS24
Friction velocity, u_*	m/s	0.44	0.41	0.405
Monin-Obukhov length, L	m	348	138	-77
Turbulent temperature scale, T_*	C	0.042	0.093	-0.159
σ_u/u_*		2.68	2.30	2.39
σ_v/u_*		3.14	1.92	2.06
σ_w/u_*		1.57	1.22	1.26
σ_T/T_*		8.81	1.85	-1.86

Sketches showing the alignment of the sensor array and the average wind direction in the FLADIS trials

FLADIS Geometry and Wind Directions - Version 1.0, 7 December 2021. Joseph Chang and Simon Gant.

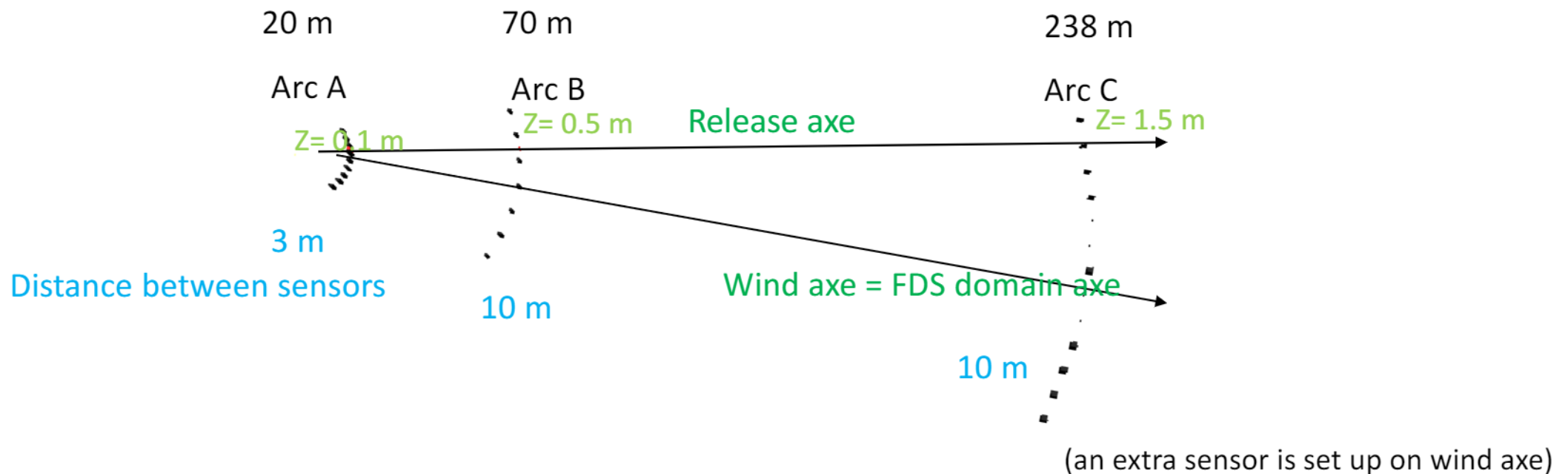


IMPLEMENTATION OF ARC SENSORS IN THE FDS DOMAIN

Flow modeling approach : Wind axis = FDS domain axis

Arc : distance from the release

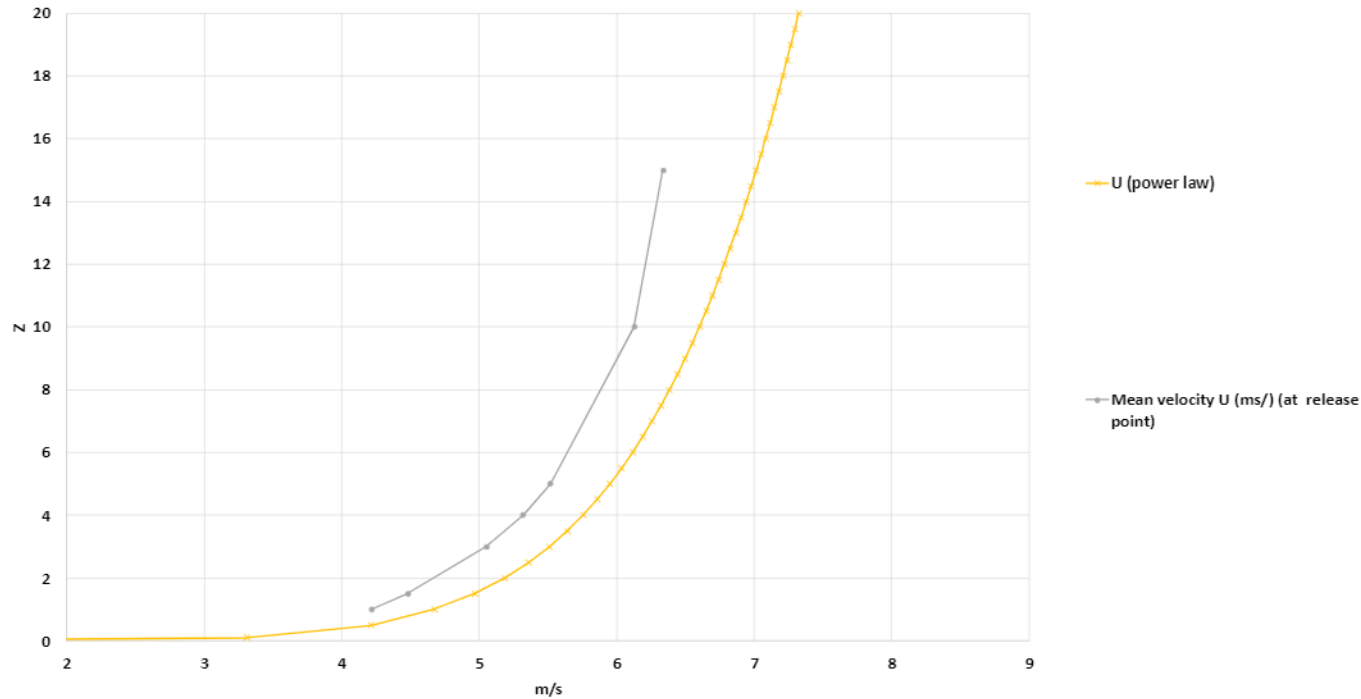
View of arc sensors by FDS



MAIN OUTPUTS

TRIAL 09: analysis of meteorological flow at release point

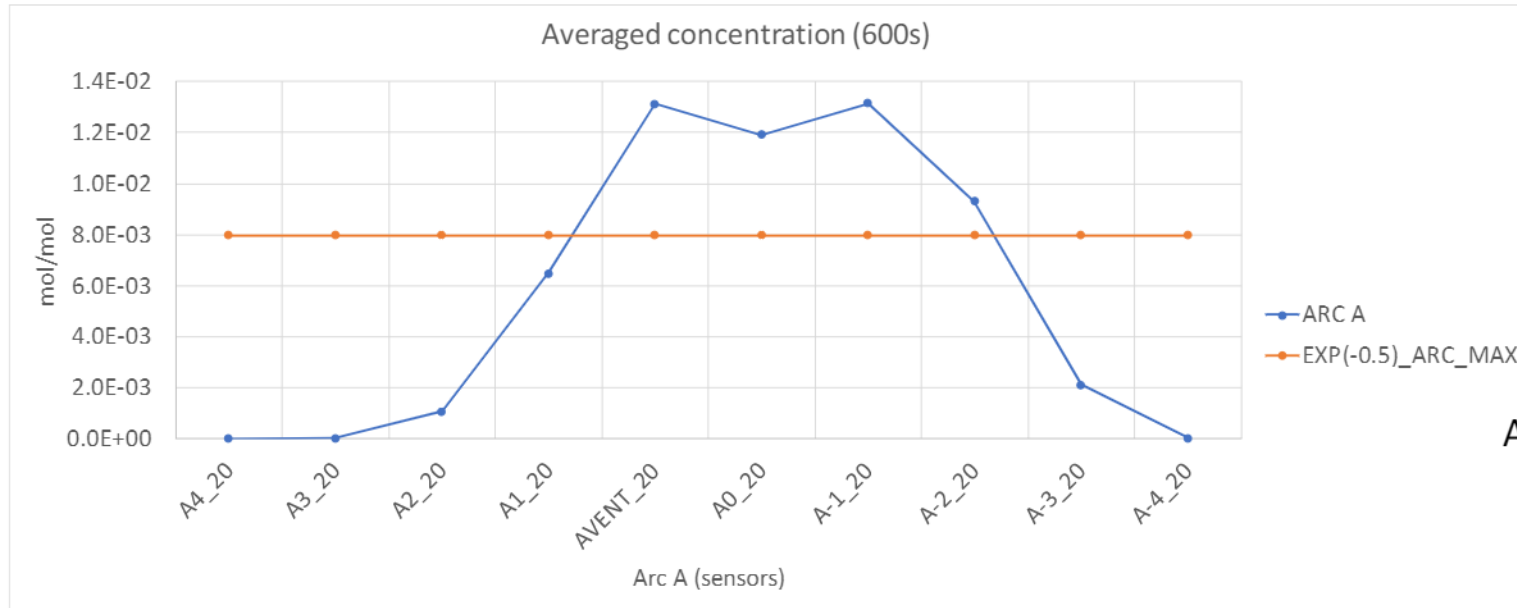
CASE 17



			u^*	$\text{sig } u/u^*$	$\text{sig } v/u^*$	$\text{sig } w/u^*$
FLADIS09 - observations			0.44	2.68	3.14	1.57
Modeling			0.33	2.55	2.17	1.16

TRIAL 09: Arc concentrations

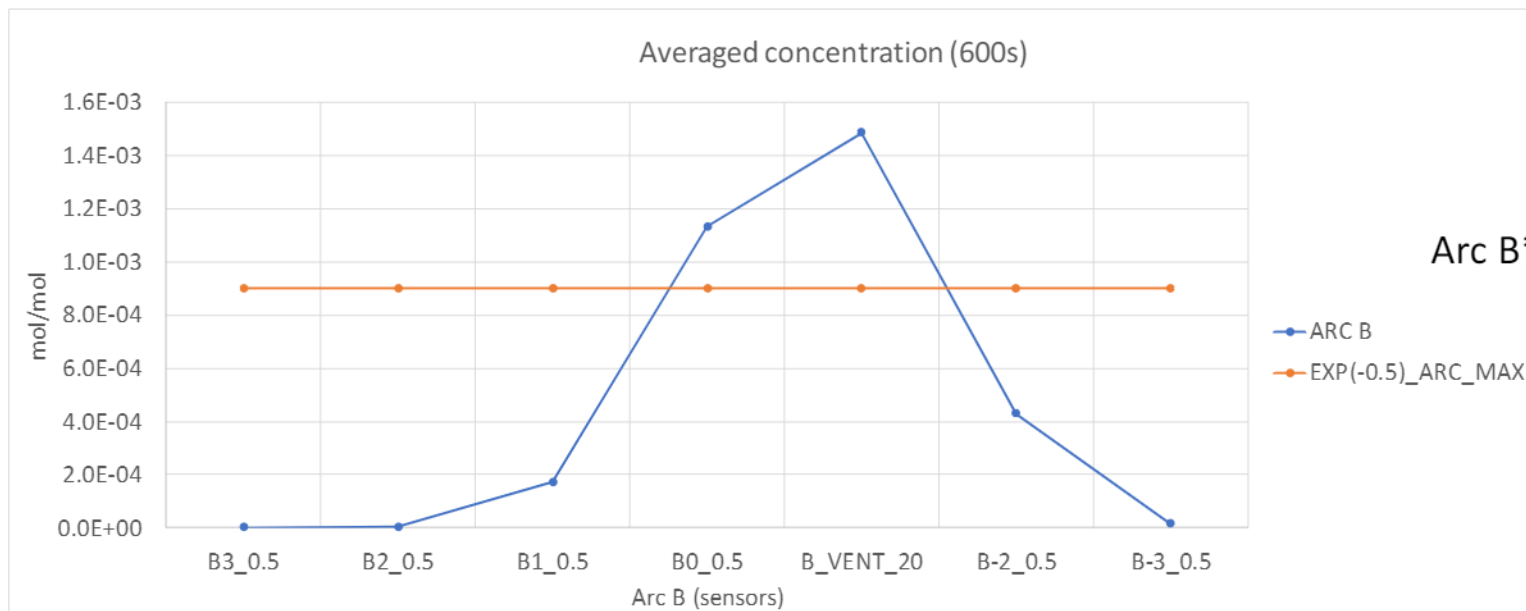
CASE 17



Rough estimate of plume width
(based upon distance between
arc sensors)



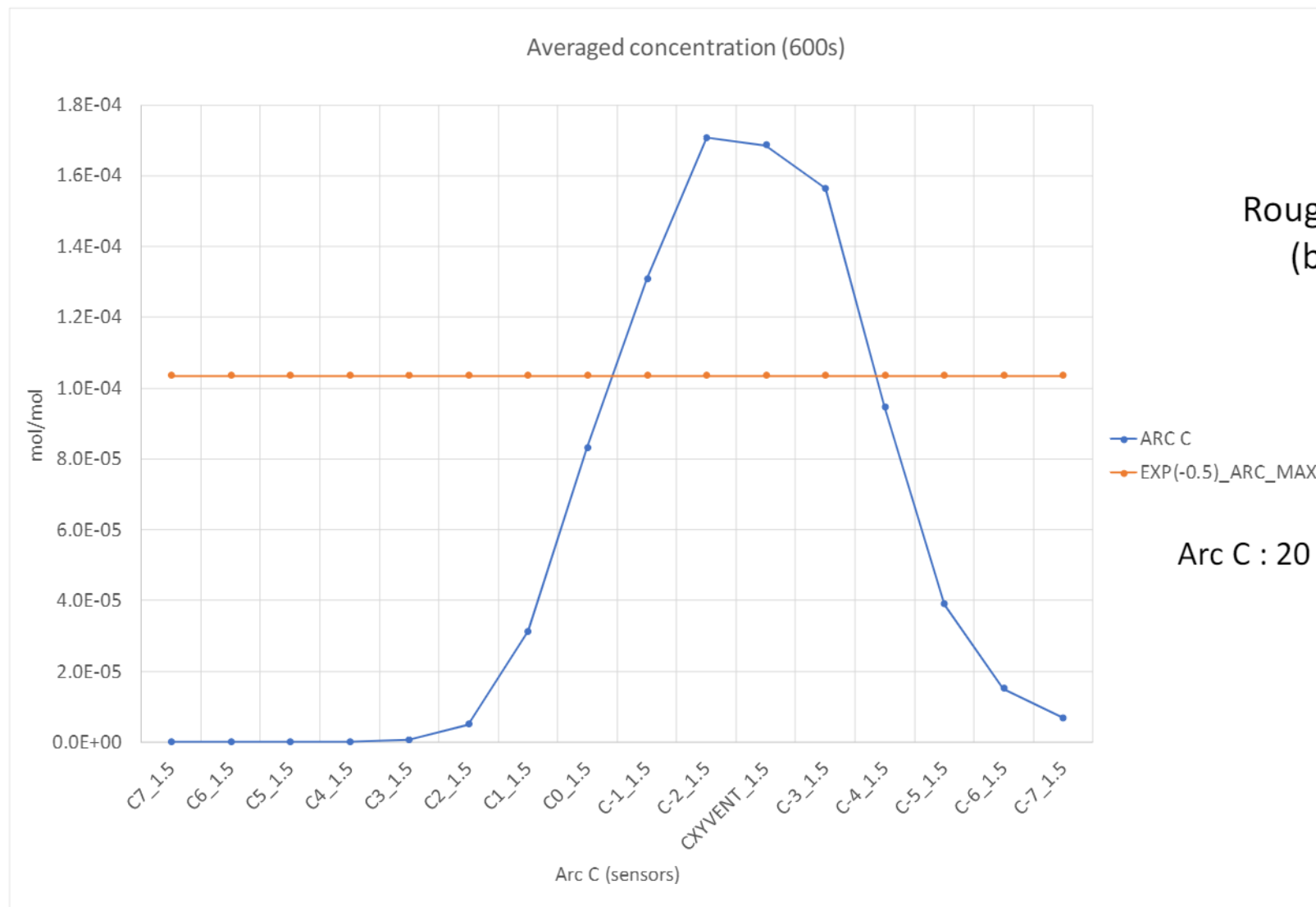
Arc A : Plume width (m) ~ 3 m



Arc B* : 10 m < Plume width (m) < 20 m

TRIAL 09 : Arc concentrations

CASE 17

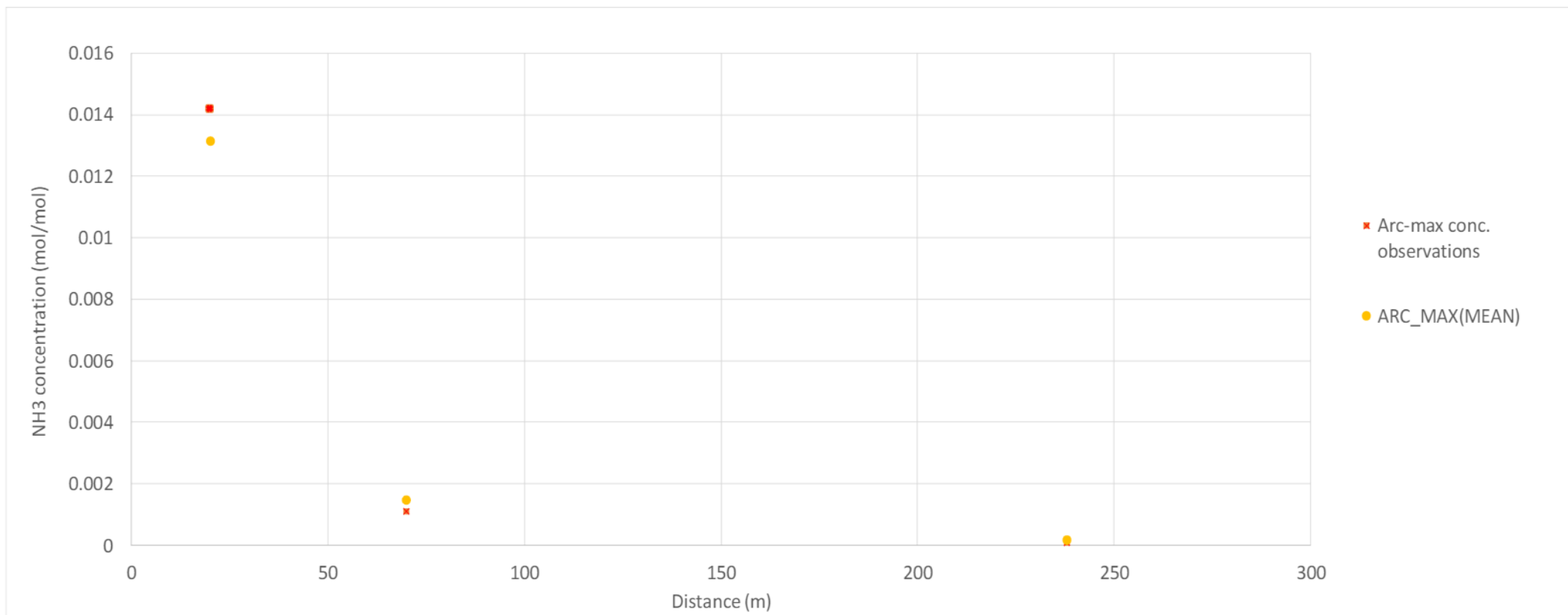


Rough estimate of plume width
(based upon arc sensors)



Arc C : 20 m < Plume width (m) < 30 m

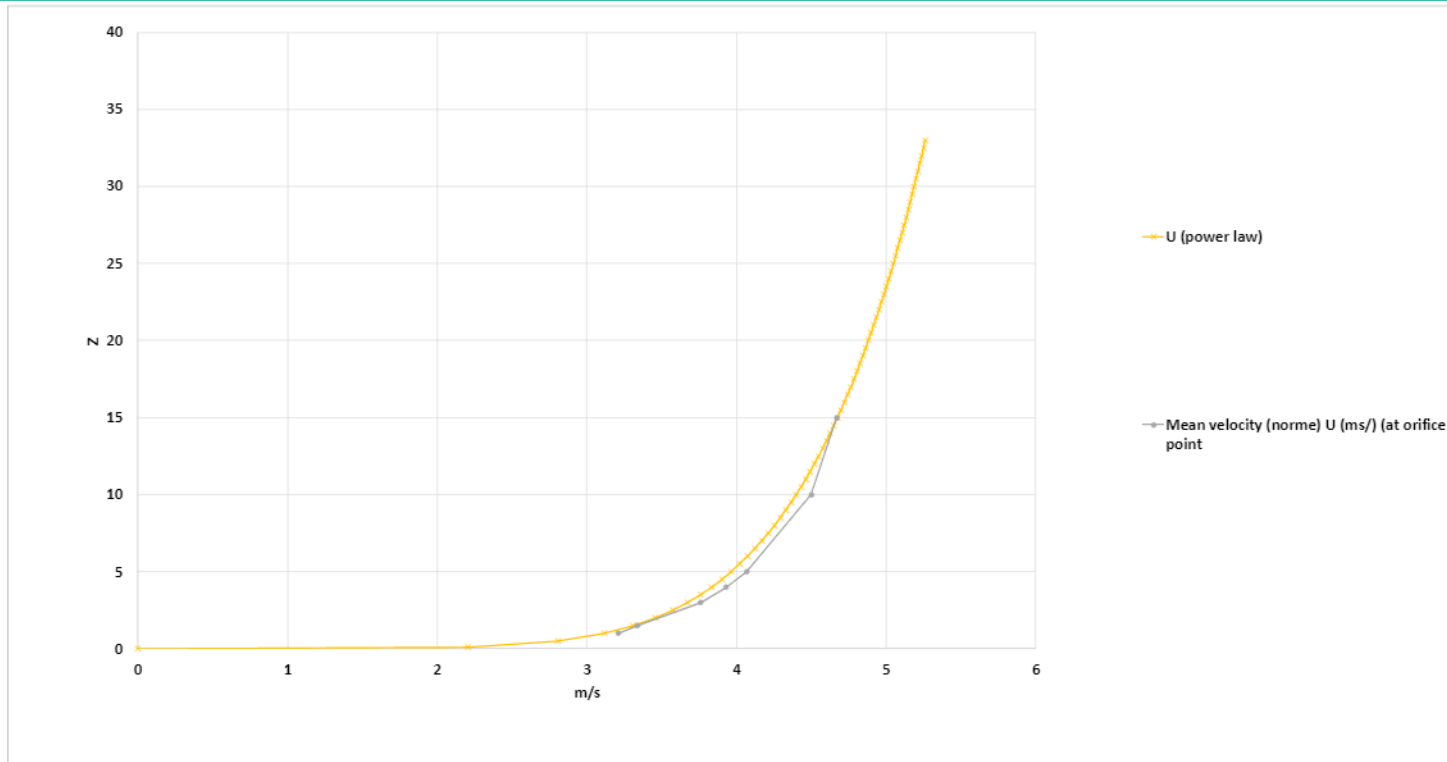
TRIAL 09 : concentrations (arc max) from the source to 300 m



Comparison Observations – Modeling

TRIAL 16 : results analysis of the meteorological flow at release point

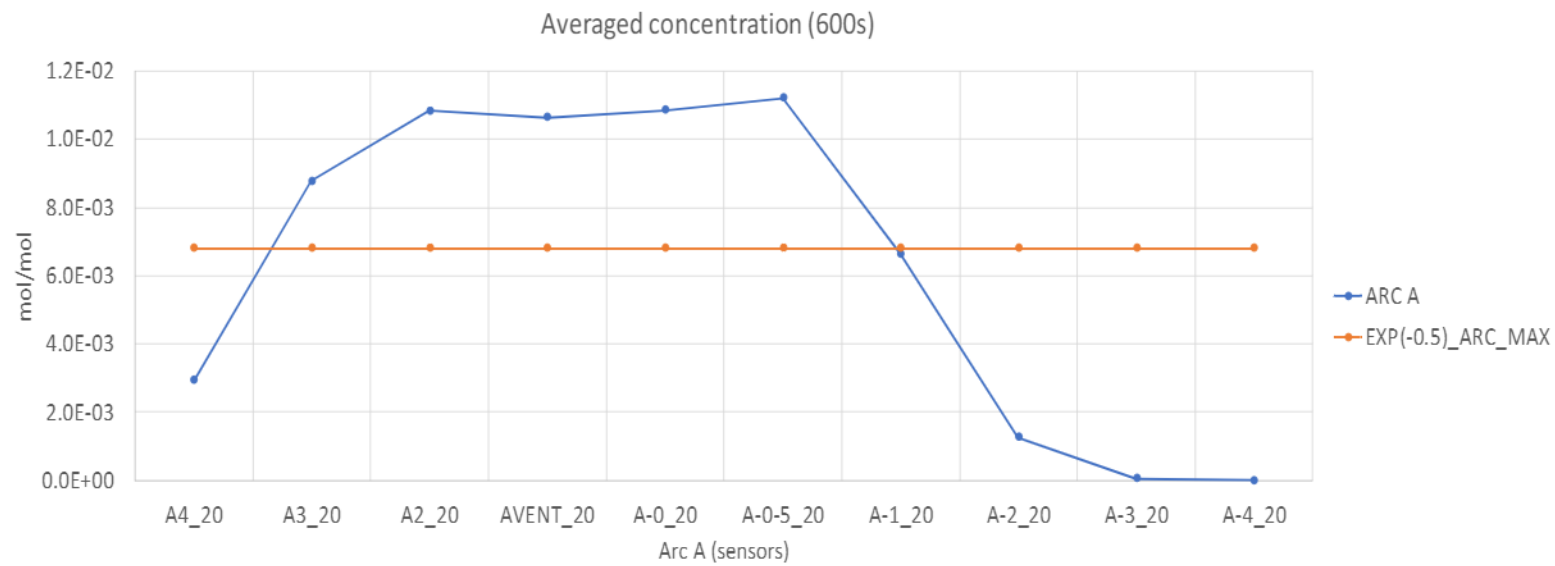
CASE 4



				u^*	sig u/u^*	sig v/u^*	sig w/u^*
FLADIS16- observations				0.41	2.3	1.92	1.22
Modeling				0.31	2.31	1.87	1.10

TRIAL 16

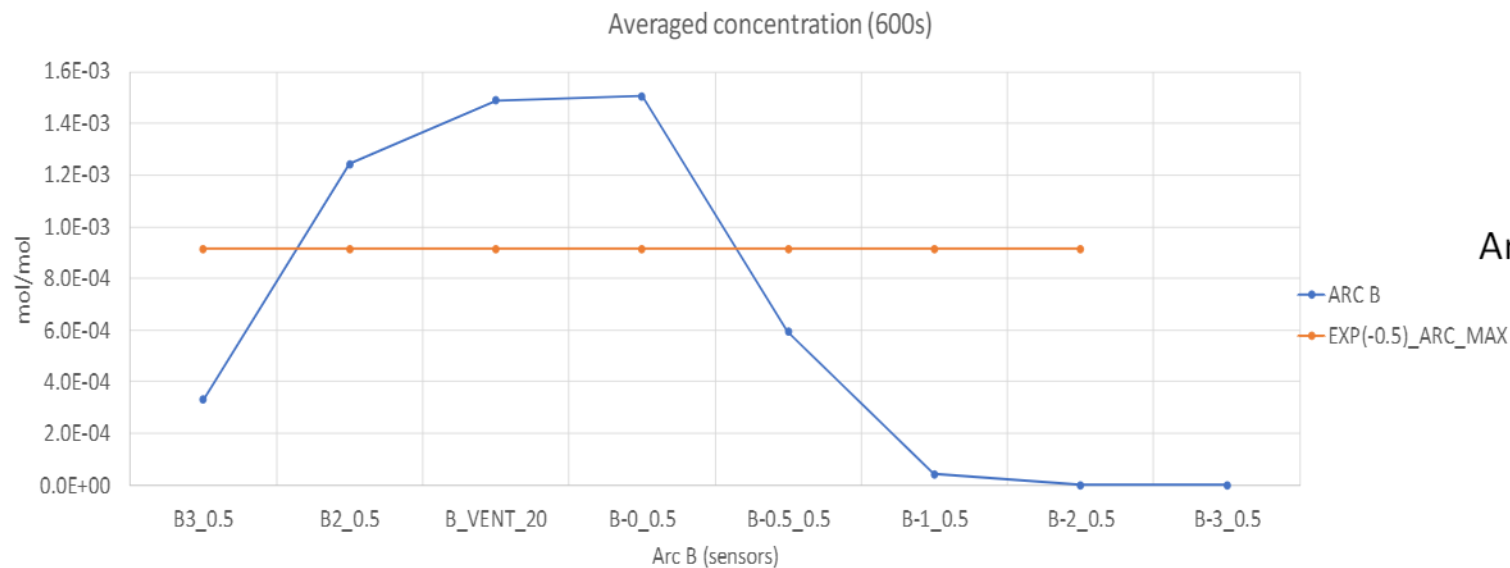
CASE 4



Rough estimate of plume width
(based upon arc sensors + one
sensor on wind direction)



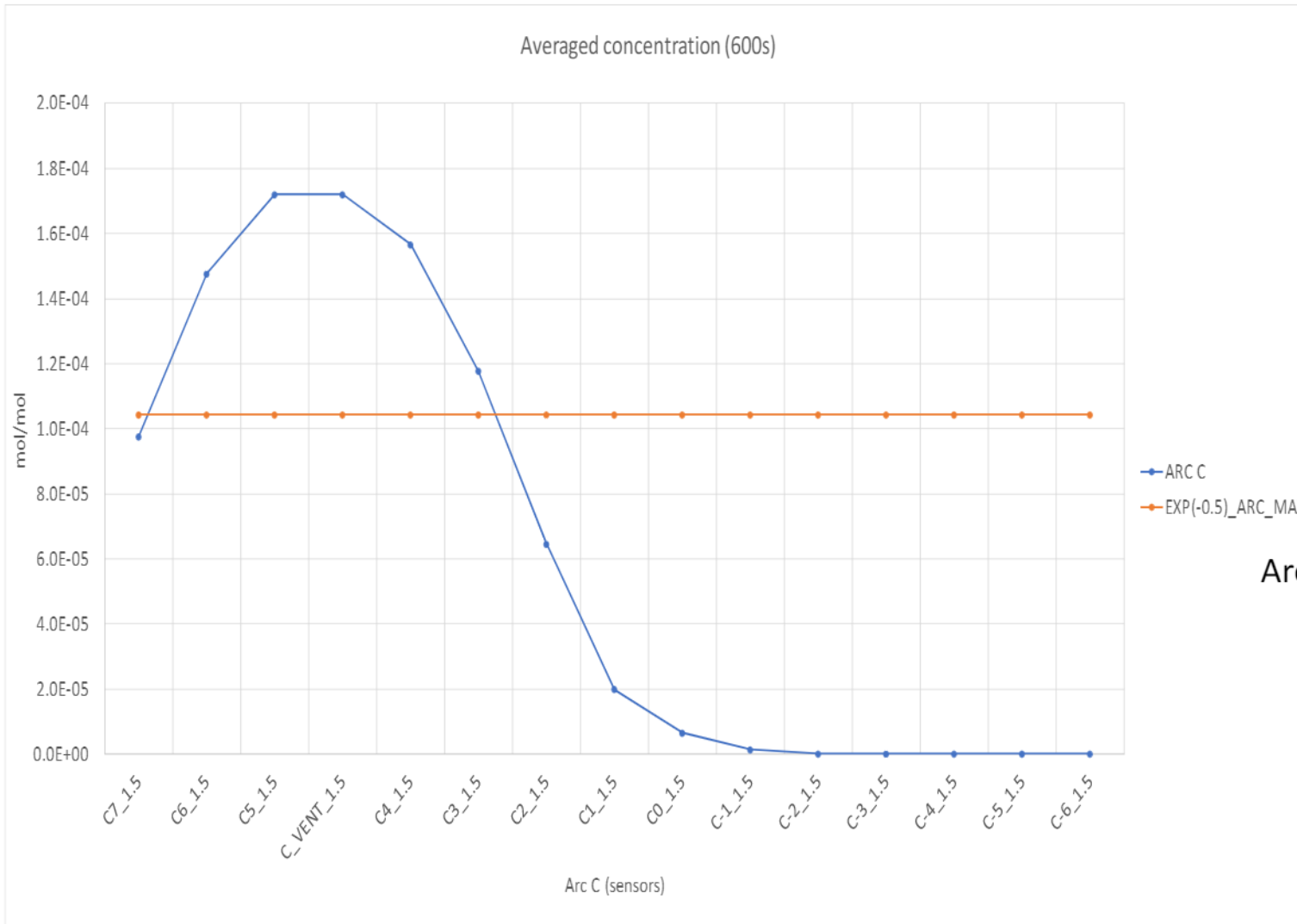
A : Plume width (m) ~ 3 m



Arc B : Plume width (m) ~ 10 m

TRIAL 16

CASE 4



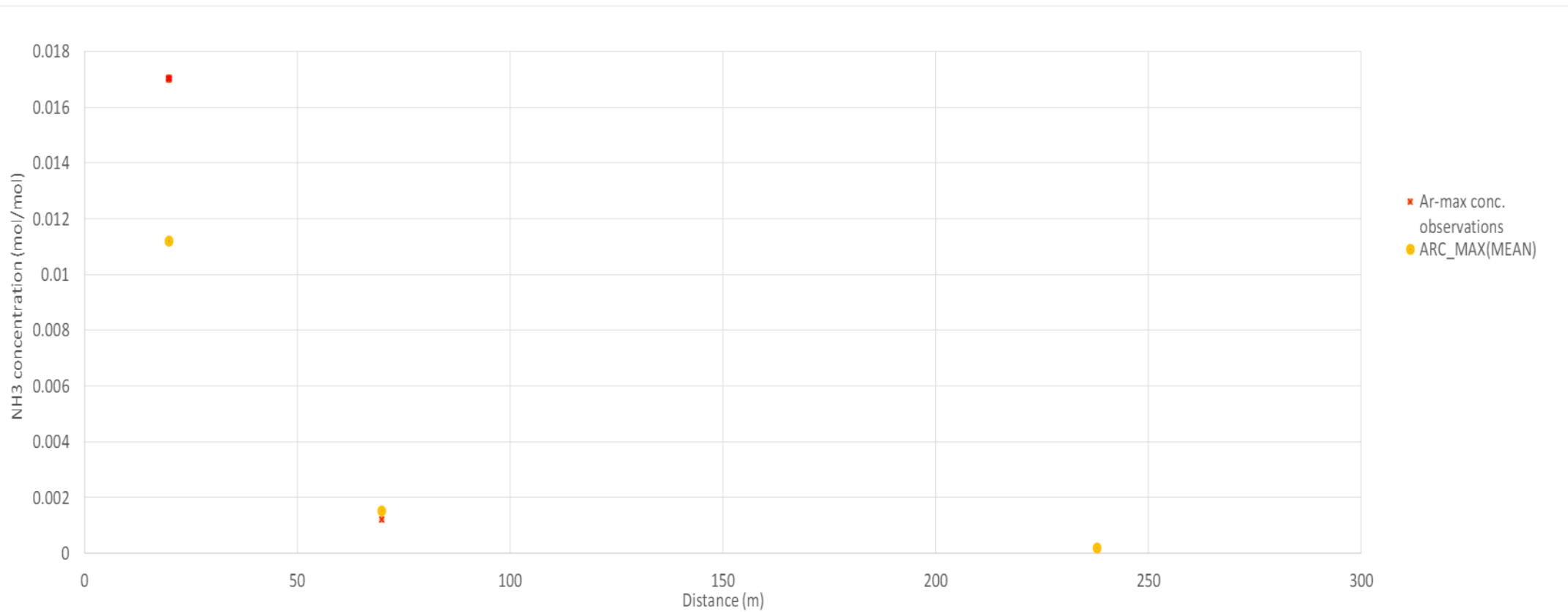
Rough estimate of plume width
(based upon arc sensors + one
sensor on wind direction)



Arc C : 20 m < Plume width (m) < 30 m

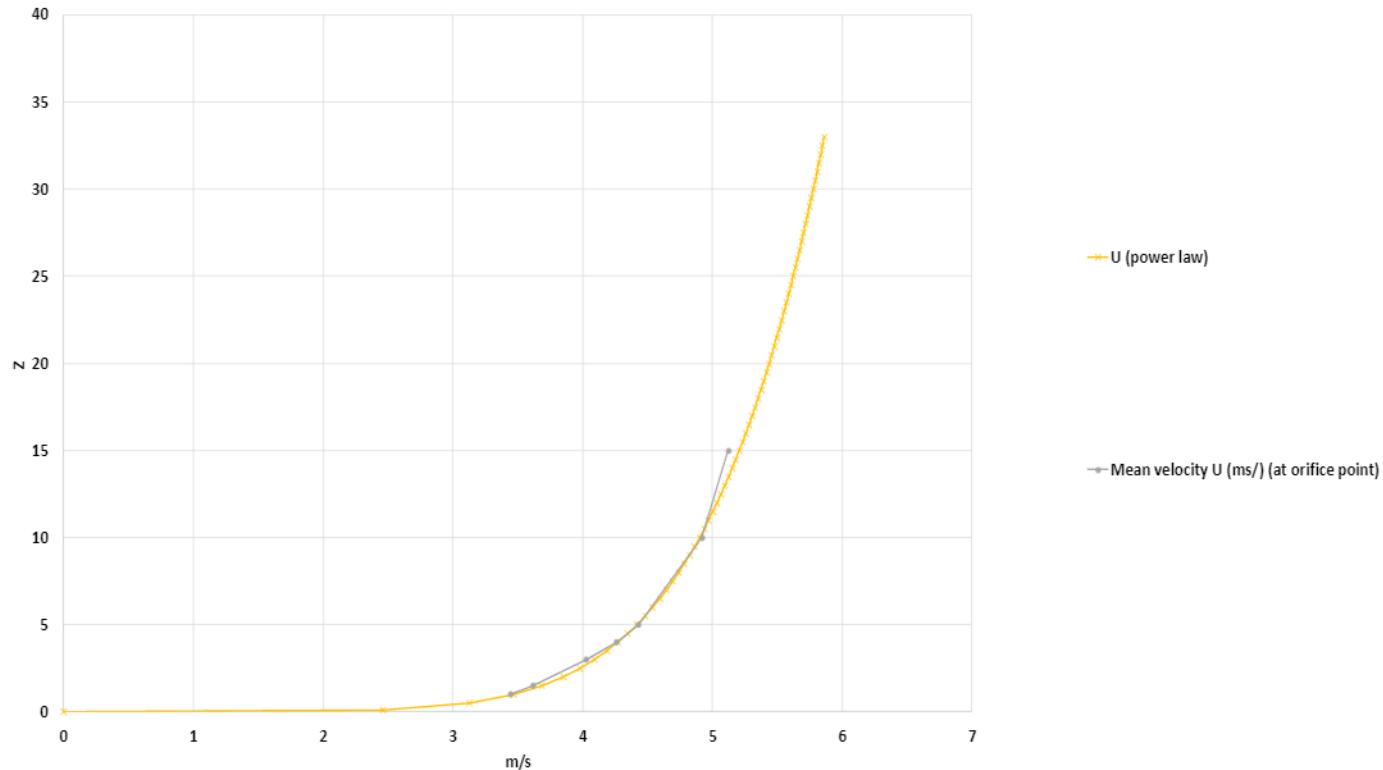
TRIAL 16 : concentrations (arc max) from the source to 300 m

CASE 4

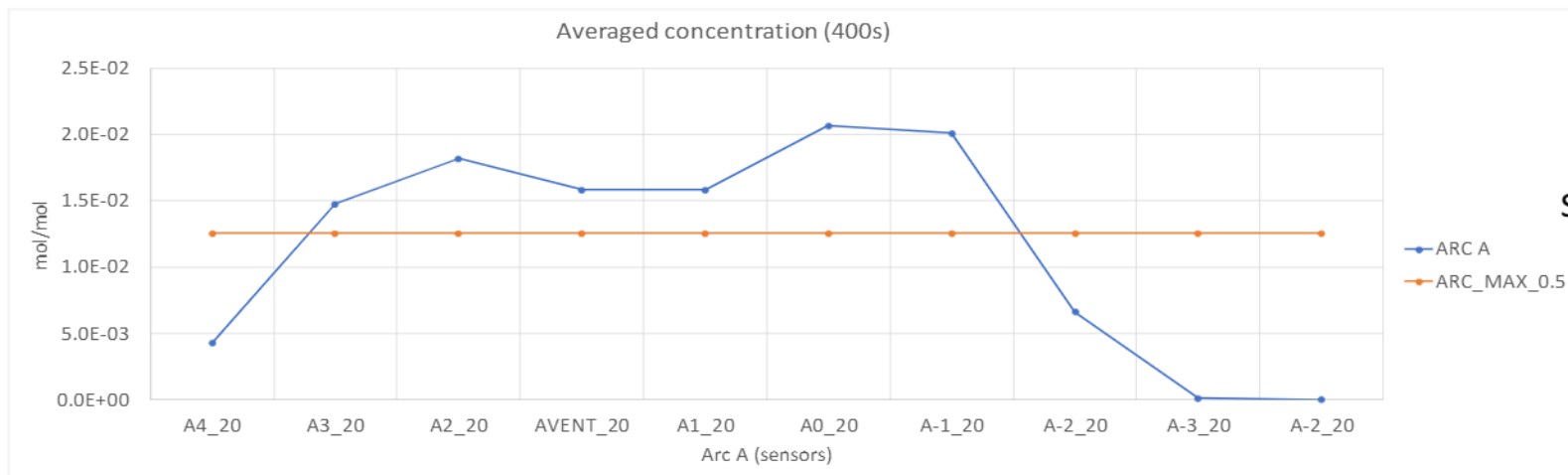


TRIAL 24 : results analysis of the meteorological flow at release point

CASE 8



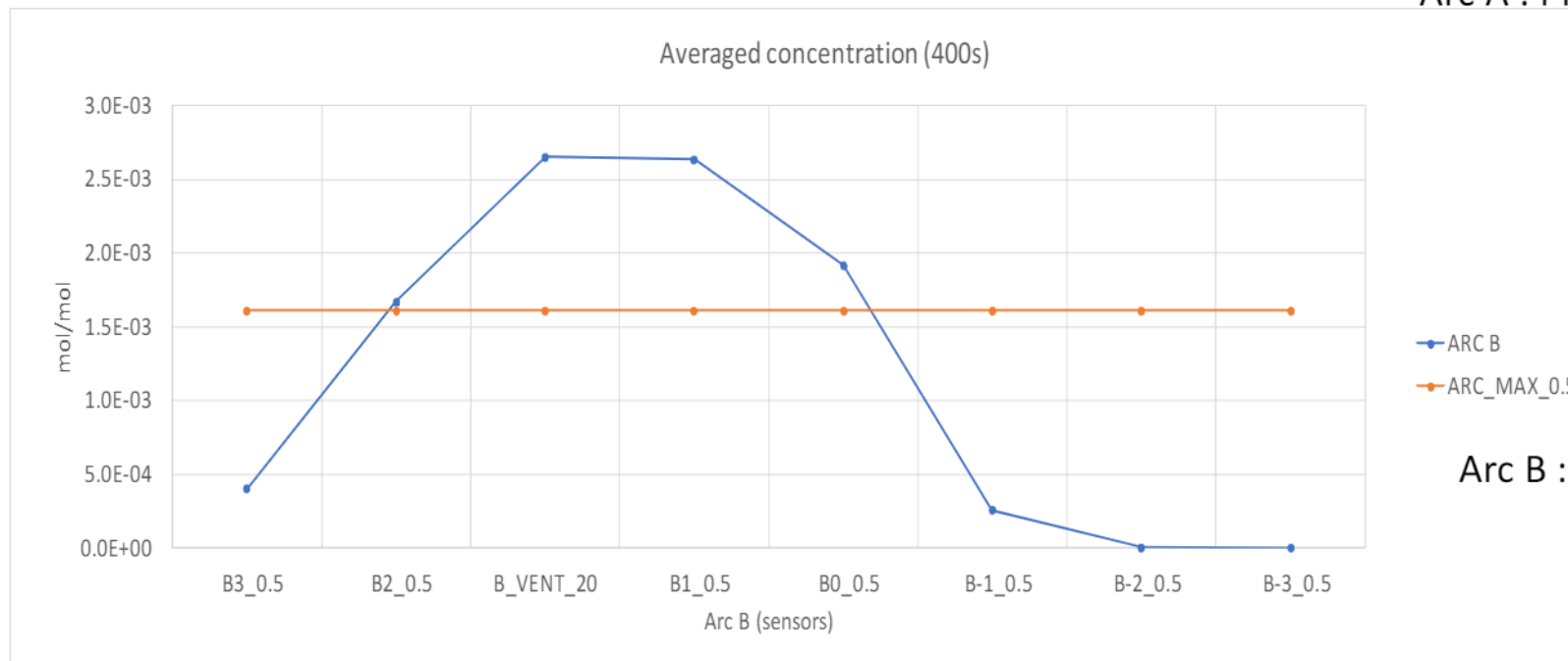
			u^*	sig u/u^*	sig v/u^*	sig w/u^*
FLADIS24- observations			0.405	2.68	3.14	1.57
Modeling			0.28	2.43	2.10	1.20



Rough estimate of plume width (based upon arc sensors + one sensor on wind direction)



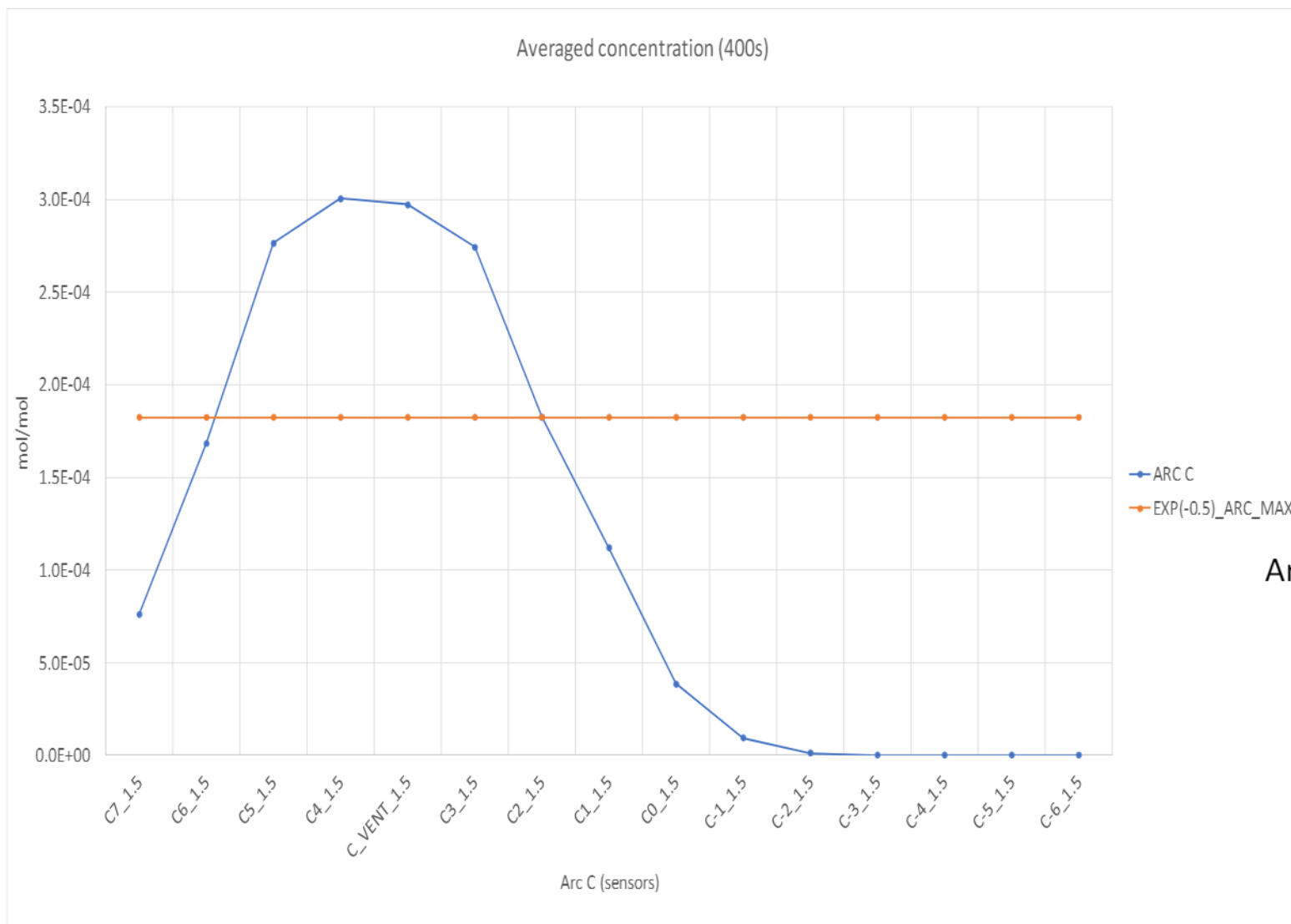
Arc A : Plume width (m) ~ 3 m



Arc B : Plume width (m) ~10 m

TRIAL 24

CASE 8



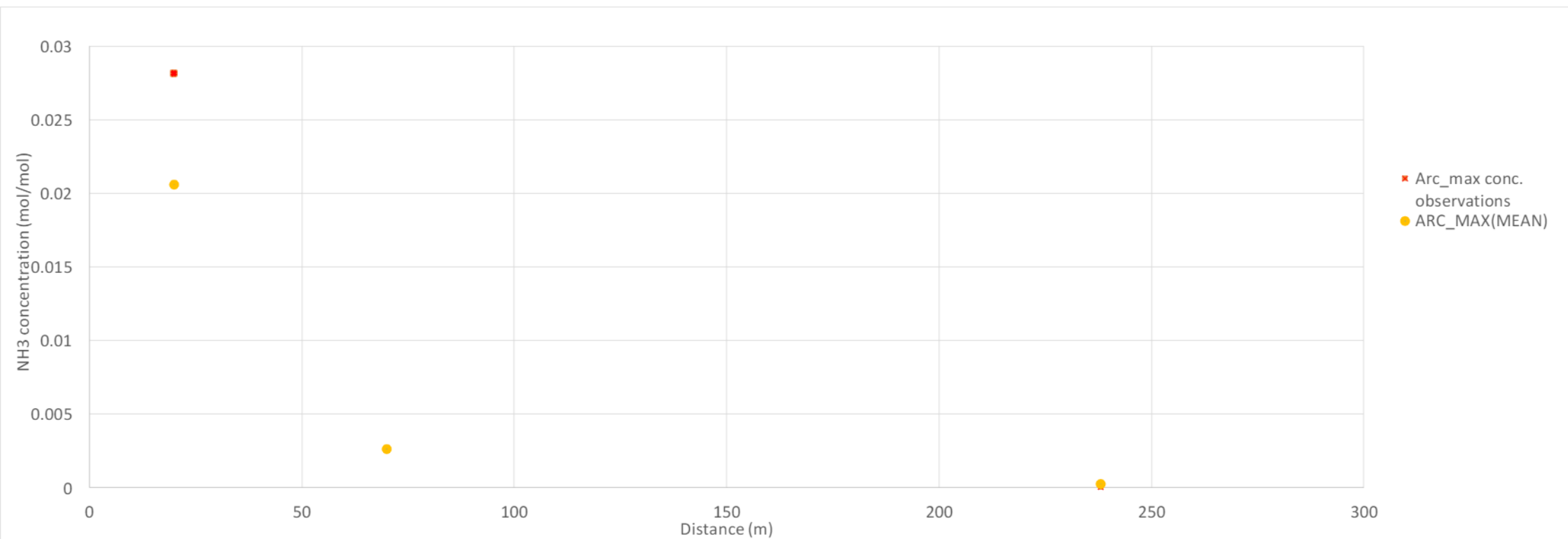
ough estimate of plume width
(based upon arc sensors + a
sensor on wind direction)



Arc C : Plume width (m) ~ 20 m

TRIAL 24 : concentrations (arc max) from the source to 300 m

CASE 8



Concluding comments

FLADIS Trial modeled by Fire Dynamic Simulator (LES approach)


Modeling of the flow and dispersion by LES approach

- / SEM precursor approach
- / Comparison of the flow mean and turbulence statistics

NH₃ release implementation by equivalent source term

Concentration Outputs

- / Average arc concentrations
- / Rough estimate of plume width
- / Concentrations (Arc max) along the distance → WG coordinator



Sincere thanks to the organizations responsible for
funding and managing the Jack Rabbit II trials and the
Jack Rabbit III Modeler's Working Group coordinators and
participants

THANK YOU FOR ATTENTION

