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CFD Simulation of Ammonia Dispersion from a Vapor Box: Secondary Containment for Handling Ammonia Spills

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Definitions

Secondary containment - a second line of defence for preventing, controlling or mitigating major hazards events. It can take a number of forms, the most common are bunds ,drip trays, expansion vessels, building structures/ventilation.

Containment in structures:

TECHNICAL BACKGROUND DOCUMENT FOR OFFSITE CONSEQUENCE ANALYSIS FOR ANHYDROUS/ AQUEOUS AMMONIA, CHLORINE, AND SULFUR DIOXIDE (EPA, 1999)

Table 6-1. Ten-Minute Building Release Attenuation Factors for Continuous Releases of Ammonia

θ* (m^3/kg)	N_v (hr^{-1})	FR_{10} (dim)	θ* (m^3/kg)	N_v (hr^{-1})	FR_{10} (dim)
10.0	0	0.07	0.5	0	0.67
	1	0.08		1	0.67
	5	0.32		5	0.67
	10	0.51		10	0.67
	20	0.71		20	0.71
	30	0.80		30	0.80
	40	0.85		40	0.85
5.0	0	0.13	0.25	0	0.83
	1	0.13		1	0.83
	5	0.32		5	0.83
	10	0.51		10	0.83
	20	0.71		20	0.83
	30	0.80		30	0.83
	40	0.85		40	0.85
2.0	0	0.29	0.05	0	0.97
	1	0.29		1	0.97
	5	0.32		5	0.97
	10	0.51		10	0.97
	20	0.71		20	0.97
	30	0.80		30	0.97
	40	0.85		40	0.97
1.0	0	0.47	0.02	0	0.99
	1	0.47		1	0.99
	5	0.47		5	0.99
	10	0.51		10	0.99
	20	0.71		20	0.99
	30	0.80		30	0.99
	40	0.85		40	0.99

* Values of θ in m^3/kg can be converted to values of θ in ft^3/lb by multiplying by 16.

Containment in structures:

1. For a continuous release, the release to air, Q_{out} (t), is set equal to the source term inside the building, Q_{in} (t). For an instantaneous release, the release to air, Q_{out}, is given by the equation:

$$Q_{out} = M \times F / V; \quad (4.3)$$

where:

Q_{out}	Source strength to the atmosphere	($kg\ s^{-1}$)
M	Mass released	(kg)
V	Volume of the room	(m^3)
F	Ventilation rate	($m^3\ s^{-1}$)

Publication Series on Dangerous Substances (PGS 3)

Guidelines for quantitative risk assessment (2005)

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Ronald L.Peterson (1993) – Vapour barriers

Vapour box- four-sided structure with an open top, for containing liquid spill or a heavier-than-air gas cloud.

Box barriers were found to be effective* in diluting the cloud in the near and far field.

- The far-field dilution is primarily due to the ability of the box to retain material and thereby reduce the effective mass release rate.
- The near field reduction is due to mass reduction and the increased dispersion due to the box structure itself.
- The box also increased the time it took material to reach a downwind receptor and increased the cloud duration.

*based on wind-tunnel results

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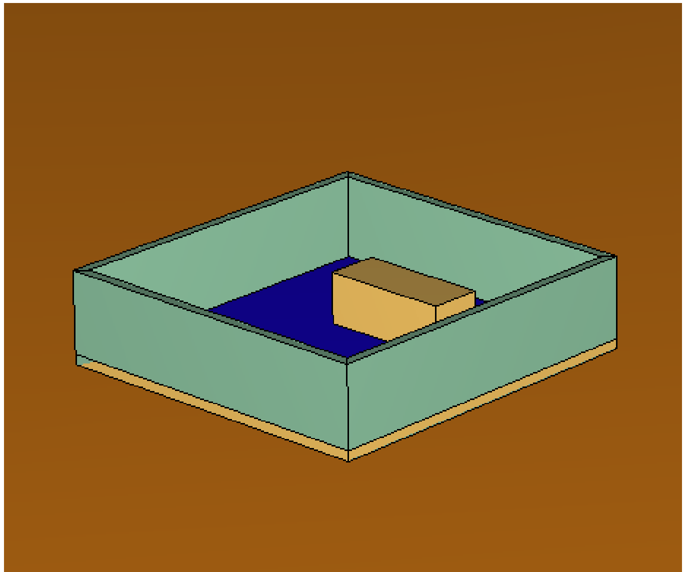
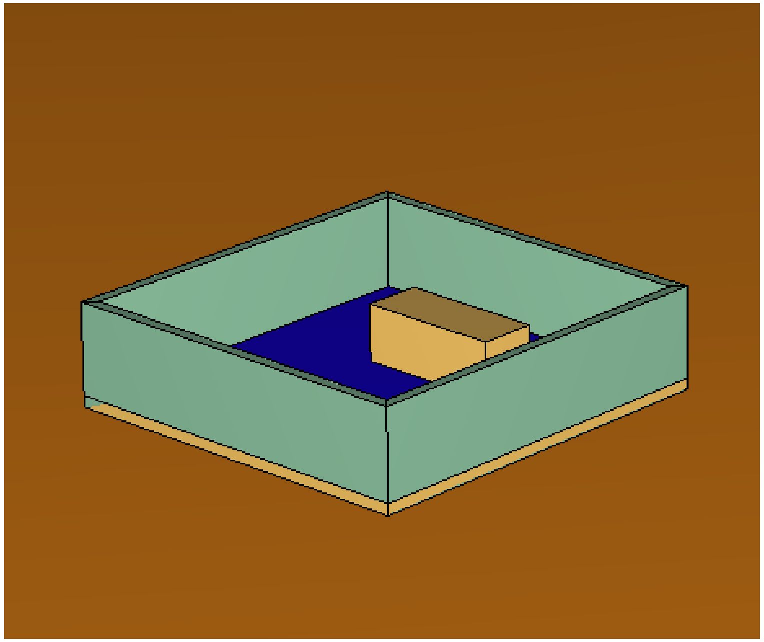
Ronald L.Peterson (1993) – Vapour barriers

<u>General guidelines for effective box performance:</u>

1. Box heights should be at or below the height of surrounding structures.
2. Box heights should be great enough such that the box volume is approximately 2 times greater than the expected release volume.
3. Box plane dimensions should be less the length of the cavity zone downwind of each box face (3 to 5 times the box height).



Spill modeling:



Vapour box with isotank inside

Reference scenario

Two inch pipe rupture of ammonia iso-tank leading to ammonia spill with EFV stopping the leak after 1 minute

Vapour box with isotank inside

Following vapour box configurations were analyzed:

[1] 30X30X5(h) with Vr/Vb≈0.5

[2] 18X18X6(h) with Vr/Vb≈1

[3] 16X16X4(h) with Vr/Vb≈2

[4] 10X10X5(h) with Vr/Vb≈5

[5] 10X10X2.5(h) with Vr/Vb≈ 9

**Vr- release volume; Vb- box volume*

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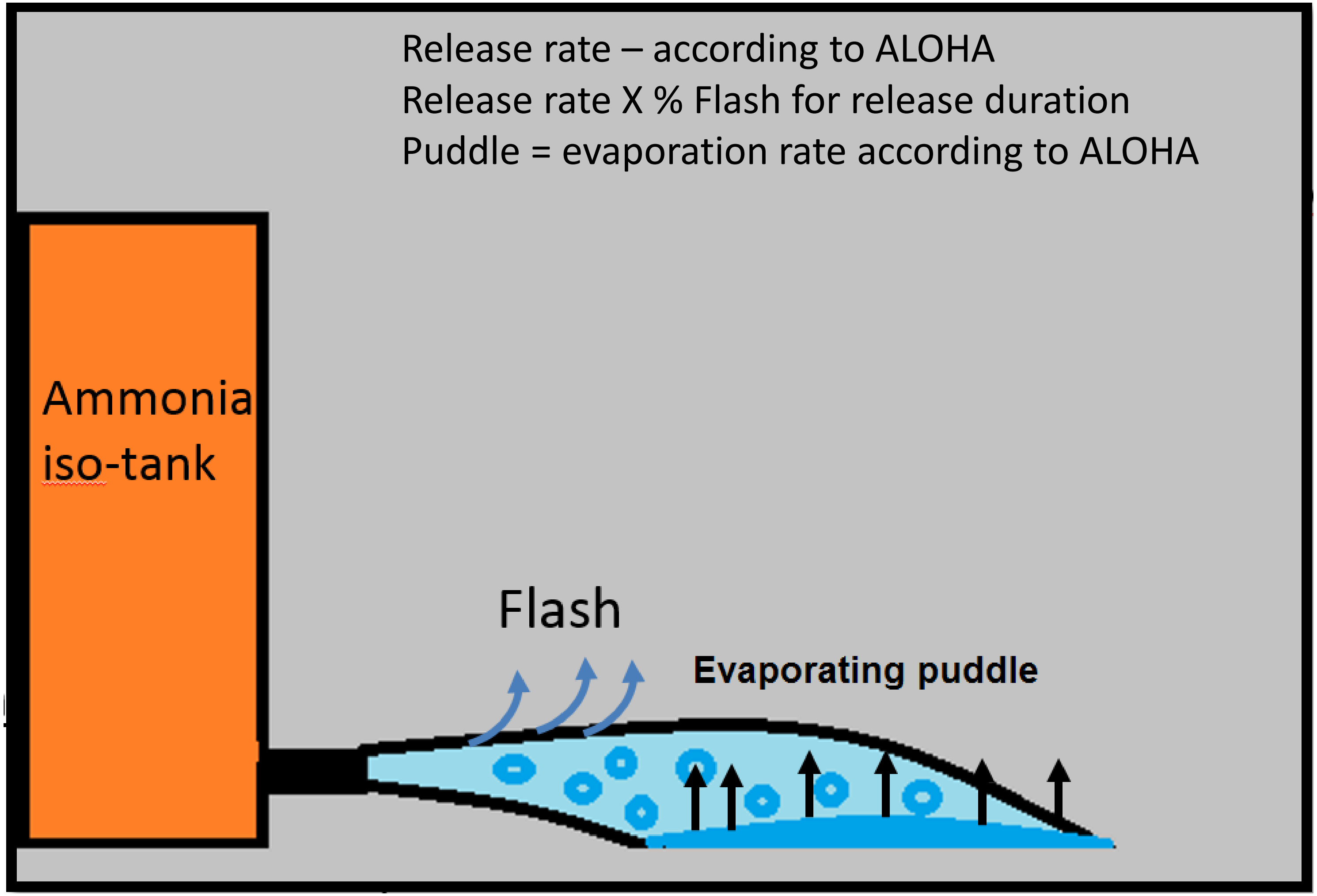
Spill modeling:



Aerosols formed during expansion cannot be directly modelled by FDS.

The ammonia vapour was injected into computational domain at a specified mass flux (flash and pool separately).

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Vapor dispersion modelling

FDS numerically solves a form of the Navier-Stokes equations appropriate for low-speed (Ma < 0.3). The chemical species equations are coupled to the Navier-Stokes equations to model the transport of chemical species.

Wind profile: Atmospheric stability is stable with wind speed varying with altitude (Monin-Obukhov similarity theory), aerodynamical roughness length z_0=0.25, temperature 10^{o}C. Open boundaries.

$$u(z) = \frac{u_*}{\kappa}\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right)\right]$$

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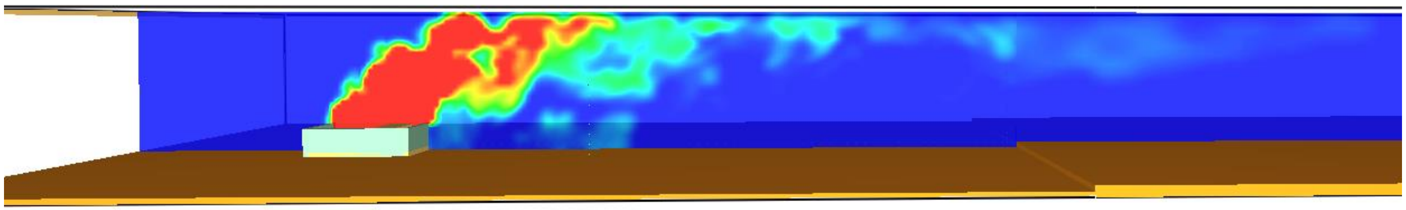
Results



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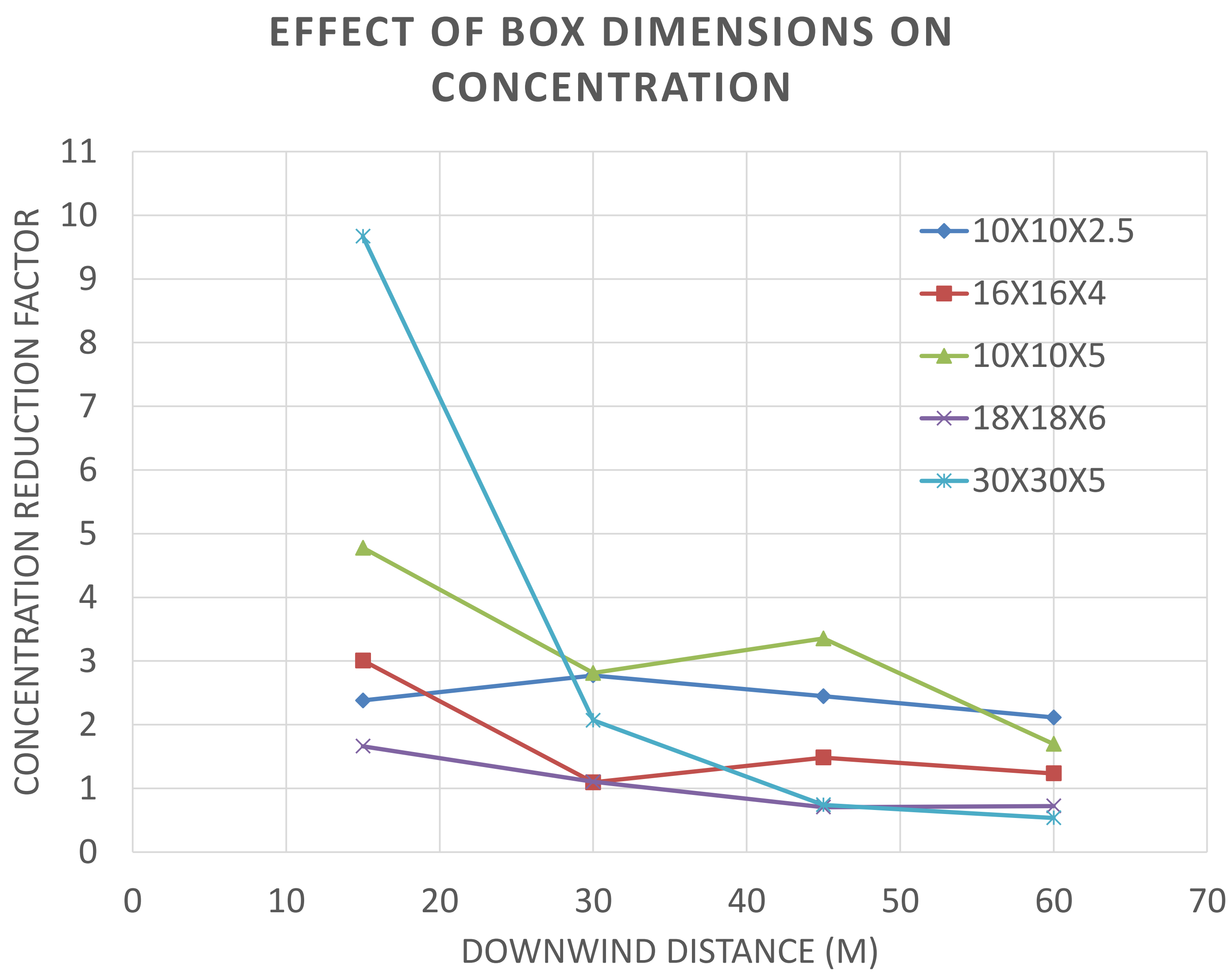
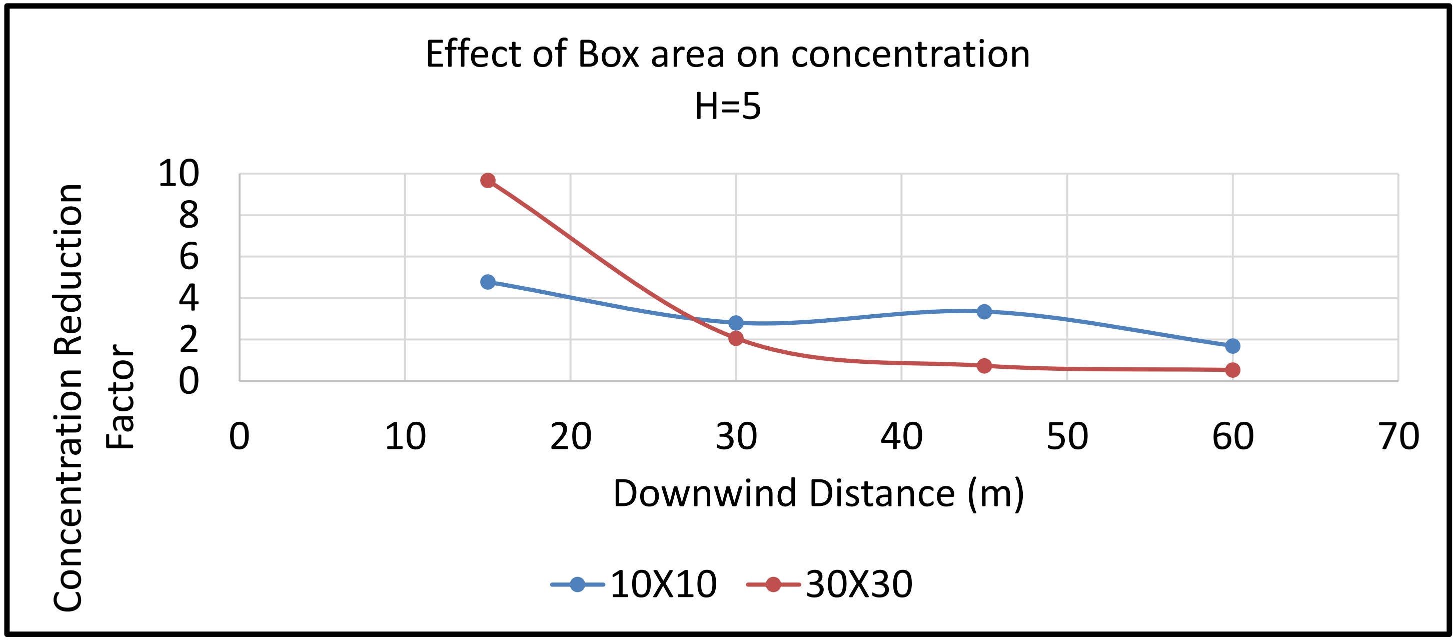
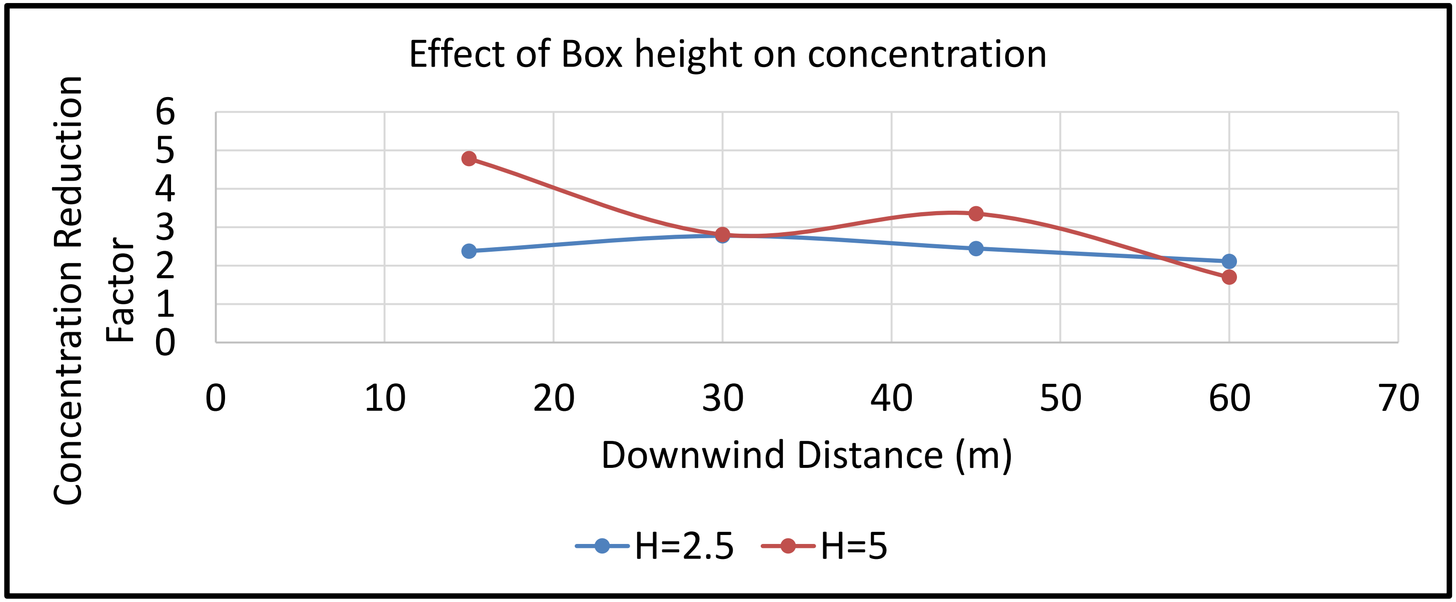
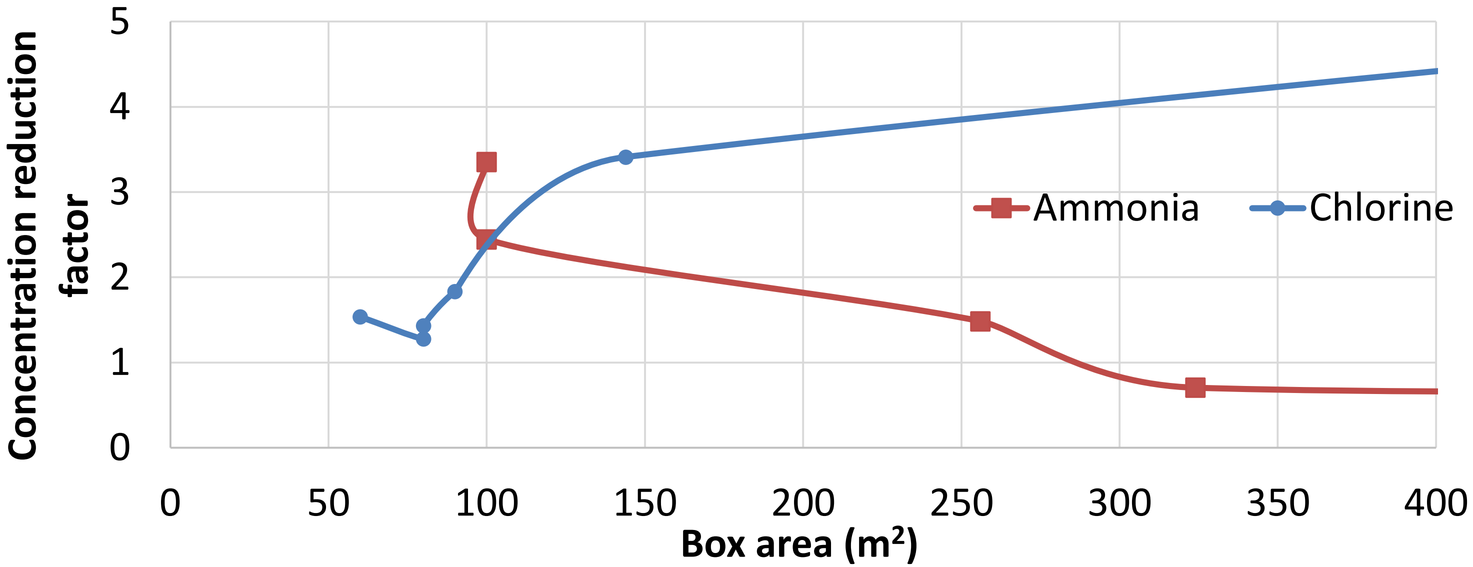
Results


EFFECT OF BOX DIMENSIONS ON CONCENTRATION
CONCENTRATION REDUCTION FACTOR
DOWNWIND DISTANCE (M)
0
1
2
3
4
5
6
7
8
9
10
11
0
10
20
30
40
50
60
70
10X10X2.5
16X16X4
10X10X5
18X18X6
30X30X5


Effect of Box area on concentration
H=5
Concentration Reduction Factor
10
8
6
4
2
0
0
10
20
30
40
50
60
70
Downwind Distance (m)
10X10
30X30


Effect of Box height on concentration
Concentration Reduction Factor
6
5
4
3
2
1
0
0
10
20
30
40
50
60
70
Downwind Distance (m)
H=2.5
H=5

Ammonia vs Chlorine



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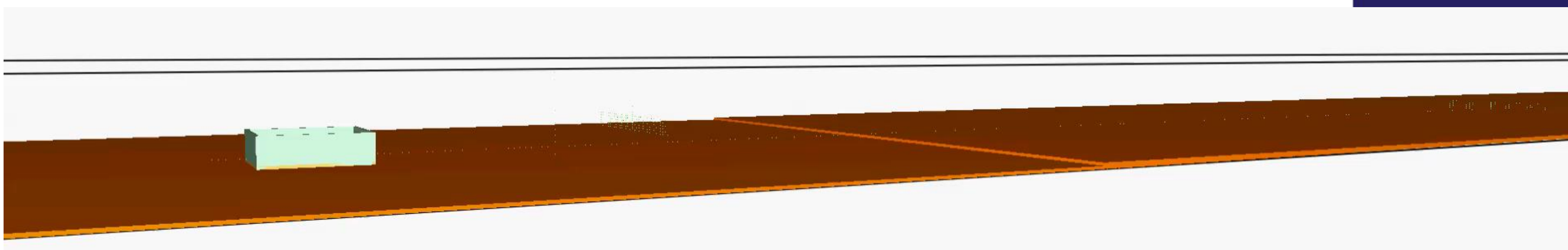
Chlorine dispersion



Discussion

- The vapor box (VB) simulation demonstrates well that the vapor box reduces effectively the risks of gas dispersion.
- The far-field effect of VB on ammonia is less significant than the effect on chlorine
- From the designer point of view, each VB requires a case-by-case study due to the complexity of the mechanism of risk reduction