#### MODITIC

Modelling the dispersion of toxic industrial chemicals in urban environments

# Comparison of various operational models against new experimental dispersion data

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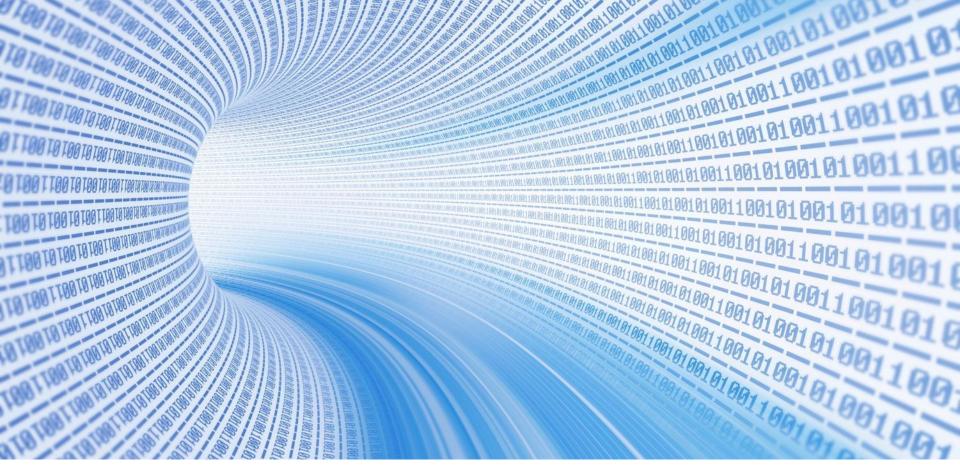












#### **OPERATIONAL MODELS**

QUIC PUMA

PMSS ARGOS

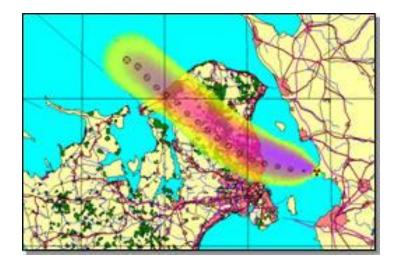


#### Goal

- To test the available operational models at hand for the contributing members of the project against new experimental data
- Not a comprising or systematic model evaluation



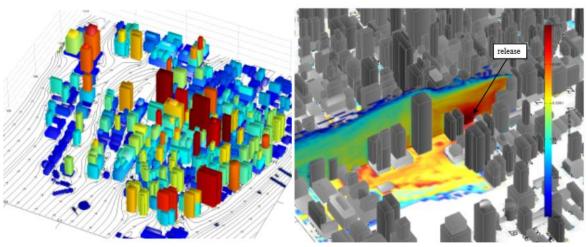
- Commercial program by PDC-ARGOS, Denmark
  - Gaussian puff model Rimpuff
  - Source estimation
  - Box model for dense gases
  - Urban wind field generator, URD, that allows for obstacles (not compatible with dense gases)





# QUIC

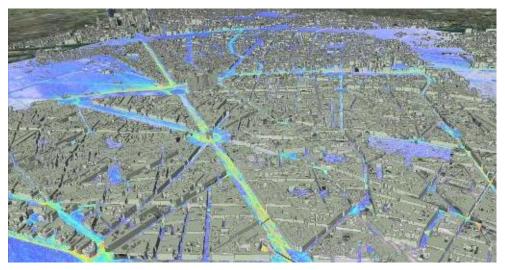
- Los Alamos National Laboratory, US
  - Quick Urban & Industrial Complex
  - Focused on urban environments
  - QUIC-URB, mass preserving flow field model
  - QUIC-PLUME, Lagrangian particle model
  - Includes a dense gas model
  - Supports multiphase releases





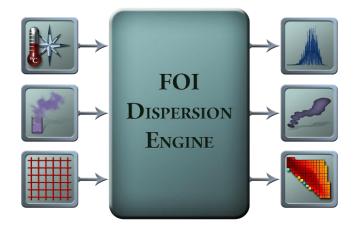
#### PMSS

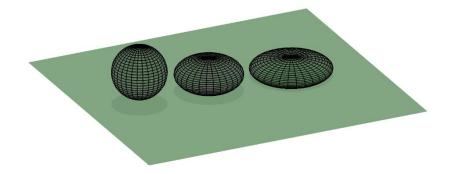
- Commercial program by ARIA Technologie, France
  - Parallel Micro-SWIFT-SPRAY
  - Micro Swift, diagnostic 3D wind fields
  - Lagrangian particle dispersion model
  - Allows for obstacles
  - Air quality monitoring
  - Dense gas module exist but was not available here



## PUMA

- PUMA is one of several models in FOIs custom made software package *Dispersion Engine*
- Puff Model of Atmospheric Dispersion
  - Real-time dispersion model
  - Designed for third-party implementations
  - Dense gas effects implemented in MODITIC

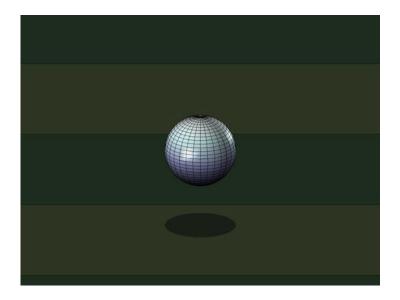


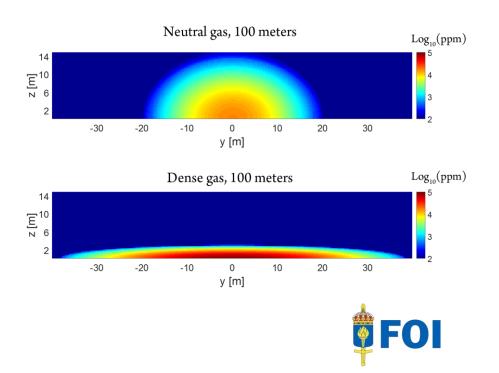




#### PUMA

- Going from neutral gas to dense gas
  - Linear  $\rightarrow$  nonlinear system
  - Geometric effects
  - Thermodynamical effects







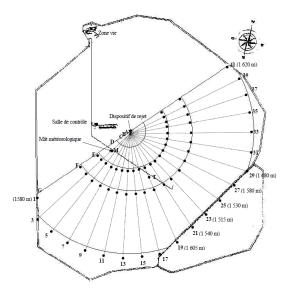
#### **CASE 1 – OPEN FIELD EXPERIMENTS**

ARGOS QUIC PUMA



# **INERIS** test site (CEA-CESTA)

- Experimental setup:
  - Ammonia, 4.2 kg/s
  - Open field, 800 meters
  - With and without a wall





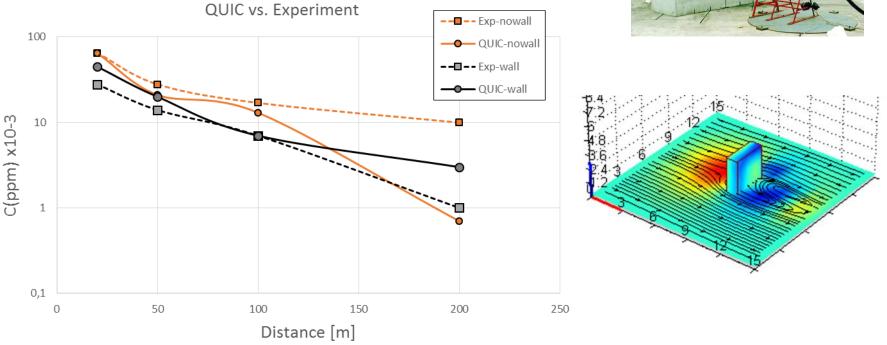




# QUIC

• With and without a wall

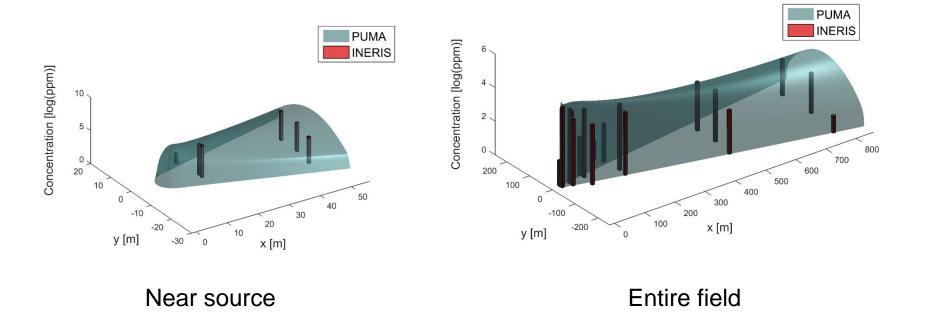






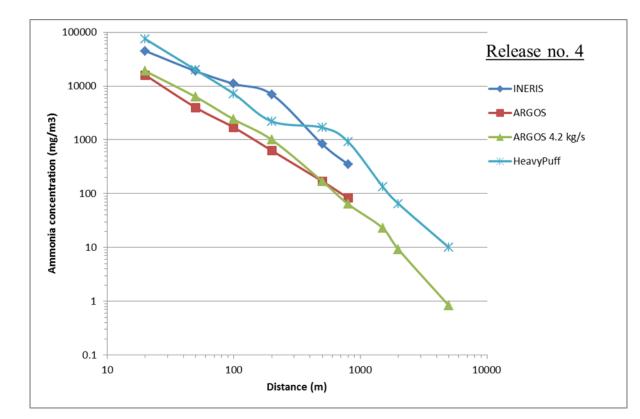
#### PUMA

• 3D fields vs. point measurements





- Comparison of both neutral and dense gas models vs. measurements – without a wall
- Also tested with an up-scaled wall

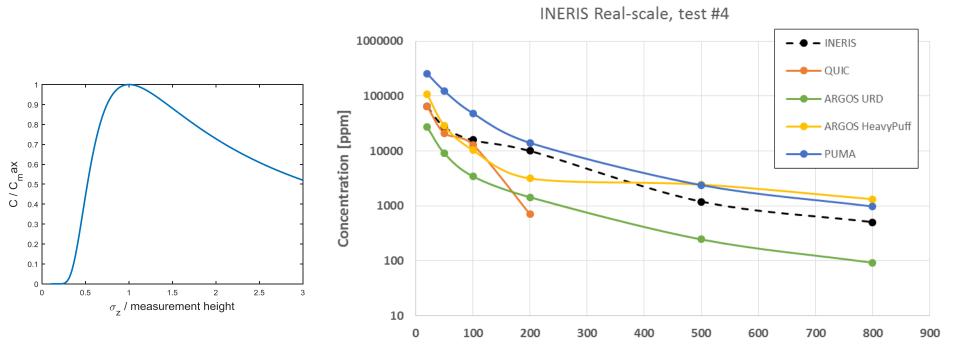


INERIS = experiment ARGOS = neutral gas HeavyPuff = dense gas



#### All models

• Plume centreline concentration at z = 1.0 meters



#### Note : Sensitive to the height!

Distance [m]

E.g., with gaussian distribution:

An increase in  $\sigma_z\!/z$  from 0.5 to 0.6 implies 53% higher C



#### **CASE 2 – PARIS WIND TUNNEL EXPERIMENTS**

ARGOS PMSS

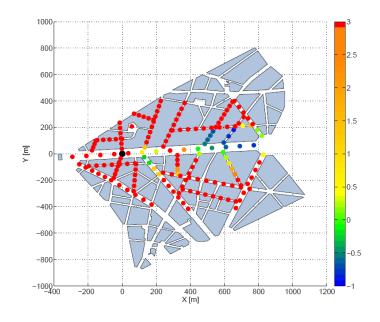


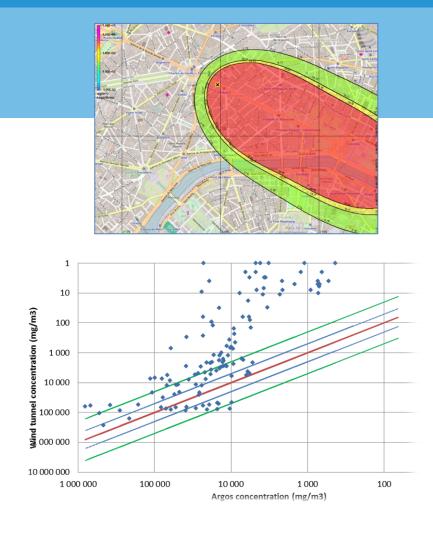


- Neutral gas only, Rimpuff & URD
- Scaled up the wind tunnel to full size, factor of 350
- Runtime a few minutes for URD



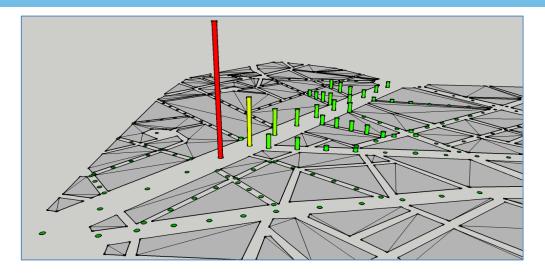
• Release point #1





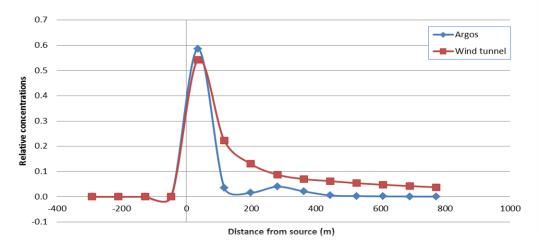
Conclusion : ARGOS underestimates the tunnelling effect of Champs Elysees and therefore overestimates the concentration outside Champs Elysees

• Release point #1



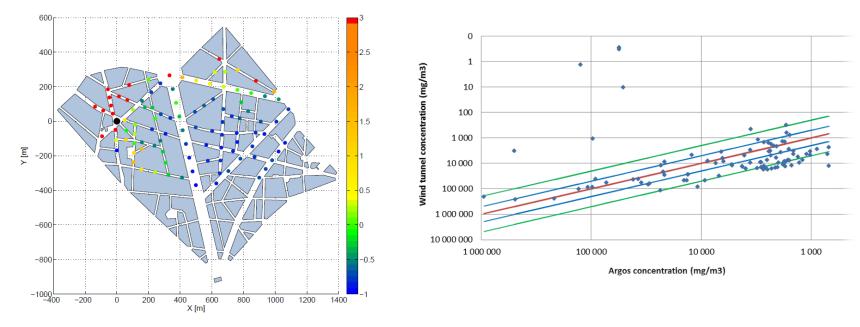
Wind tunnel data

F(



Relative concentrations along Champs Elysees

#### • Release point #3



Source position	Fraction within FAC2	Fraction within FAC5
1	0.08	0.26
2	0.18	0.47
3	0.30	0.69

Conclusion : Better results without any 'tunneling', but overestimation close to the source

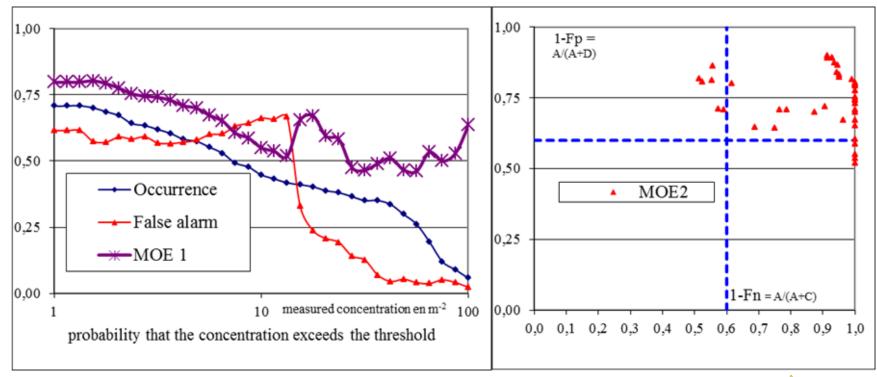


#### PMSS

Occurrence False alarm

MOE 1 MOE 2

- = how many points that exceed the threshold for measurement
- = fraction false positive
- = how large fraction of the total area that overlap
- = false positive vs. false negative for each threshold





#### Conclusions

- We have tested 4 models
- Two different main geometries open field & urban
- Dense gas and neutral gas
- ... but not all combinations!
- Only QUIC could be tested in all cases



# Conclusions

- Setting up sources and meteorology might be timeconsuming
- Execution time is short, seconds minutes
- Results:
  - Open field : No strong general trend in the results
    - HeavyPuff in ARGOS gives results closer to experimental data than Rimpuff
  - Urban : Hard to catch the strong effect of Champs Elysees.
    Overestimation close to the source.

Full report: Burkhart, S., Gousseff, A., Tørnes, J., & Björnham, O. 2016. MODITIC - Simulation Report on Operational Urban Dispersion Modelling

