



# Gas dispersion in atmospheric boundary layers

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- Simulation of gas dispersion in urban environment with OpenFOAM
- Prediction e.g. for toxic and flammable gases
- Very complex underground
- Area upstream of dispersion should be resolved
- Reduce inlet length (synthetic turbulence at inlet)
- No precursor or recycling needed (less computational costs)



\*



- Using rhoReactingBuoyantFoam solver
- Conservation equations

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{U}) = 0 \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{U}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{U} \tilde{U}) = -\nabla \bar{p} + \nabla \cdot (\tilde{\tau}_{\text{eff}}) + \bar{\rho} g \quad (2)$$

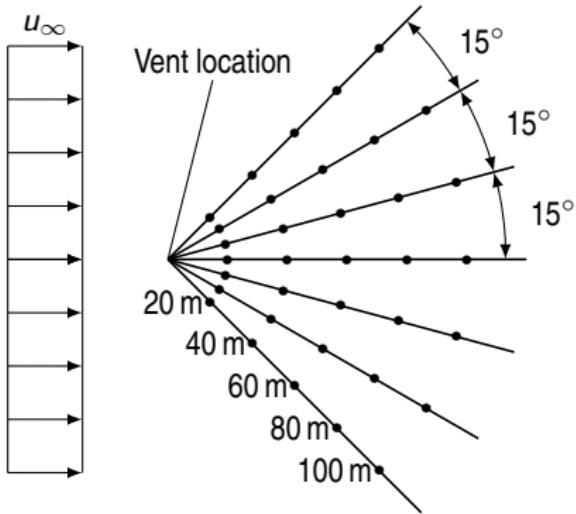
$$\frac{\partial \bar{\rho} \tilde{Y}_i}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{U} \tilde{Y}_i) = +\nabla \cdot (\mu_{\text{eff}} \nabla \tilde{Y}_i) + \bar{S}_y \quad (3)$$

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{U} \tilde{h}) + \frac{\partial \bar{\rho} K}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{U} K) = -\nabla \cdot (\alpha_{\text{eff}} \nabla \tilde{h}) + \bar{S}_h \quad (4)$$

- With additional initialization of p\_rgh field
- Little changes in pressure correction for stability reasons



## Description of first test case



†

† Jennifer Wen u. a. "Dispersion of carbon dioxide from vertical vent and horizontal releases—a numerical study". In: *Proceedings of the Institution of Mechanical Engineers, Part E: Journal of Process Mechanical Engineering* 227.2 (2013), S. 125–139.



## Description of first test case



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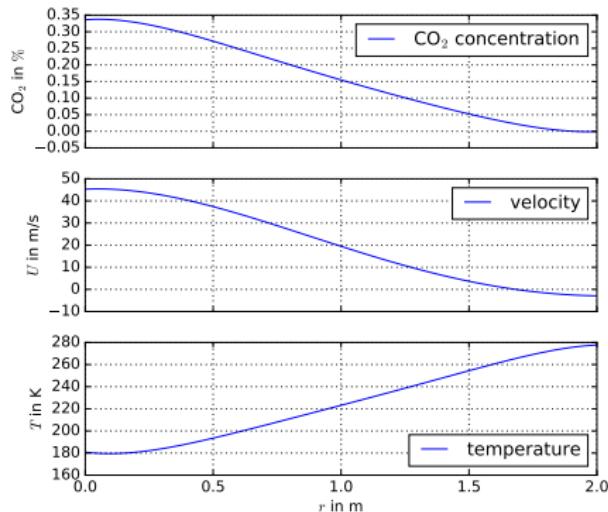
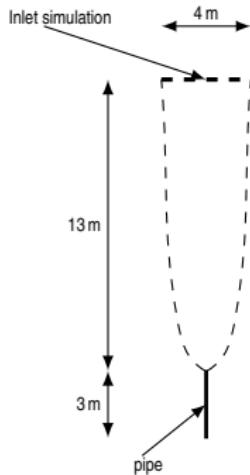
- Dispersion of CO<sub>2</sub> from jet (20 s inflow)
- Pure CO<sub>2</sub> at the outlet
- Vent with D = 50 mm at 3 m height
- Pressure in CO<sub>2</sub> vessel 151 bar
- Wind velocity at 2 m height ≈ 1,8 m/s
- Measurements of CO<sub>2</sub> concentration downstream at 1m height

\* Wen u. a., "Dispersion of carbon dioxide from vertical vent and horizontal releases—a numerical study".



## Description of simulation

- Profiles for T, U, CO<sub>2</sub>-fraction in 13 m above pipe (from <sup>†</sup>)

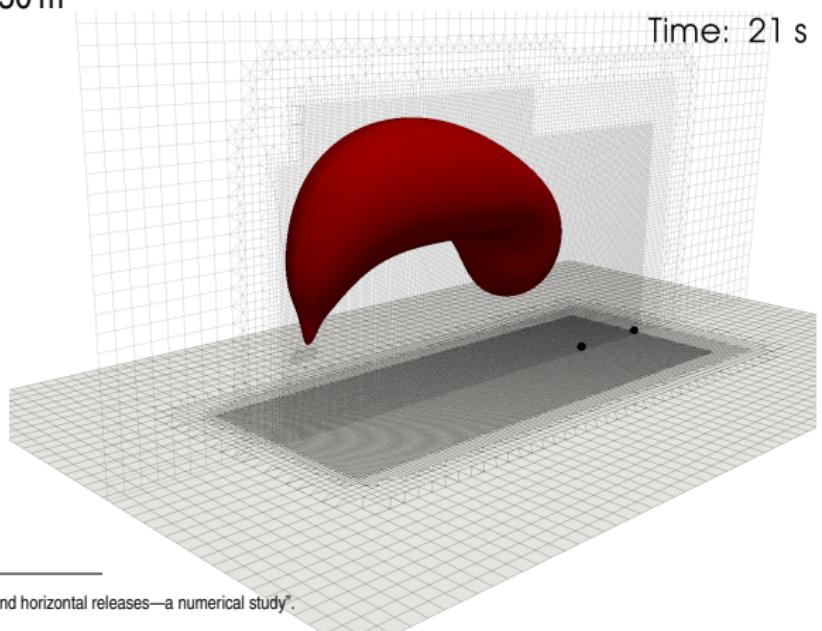


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## Description of simulation

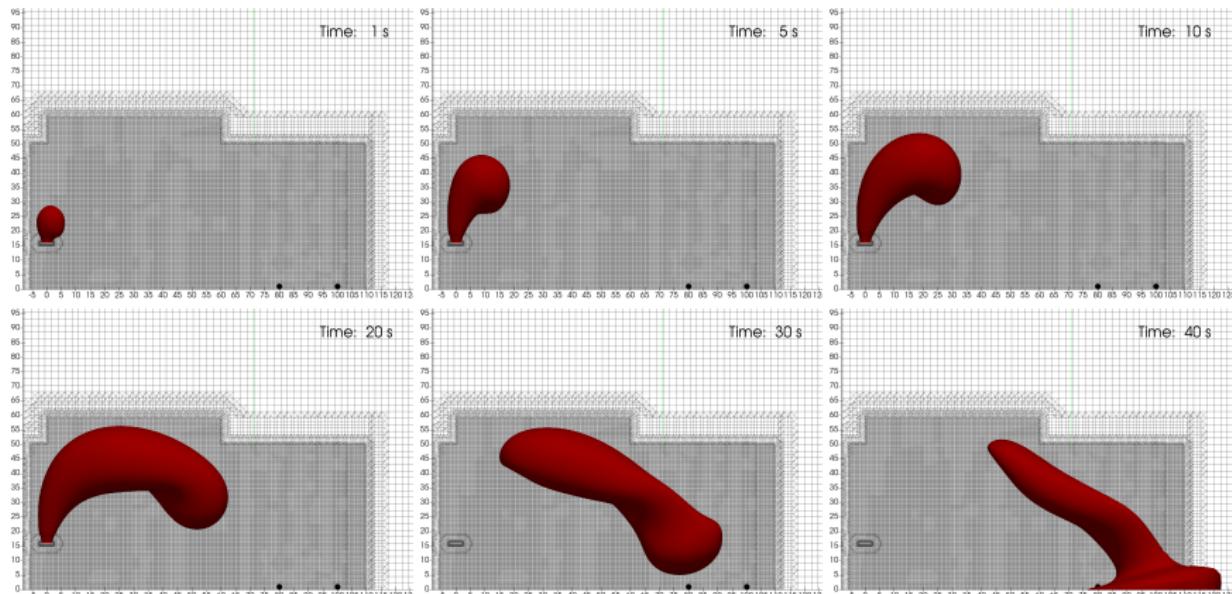
- RANS with constant atmospheric boundary layer profile ( $z_0 = 0.01$ , suggested in <sup>†</sup>)
- Domain 190 m x 120 m x 150 m
- Mesh size 1M to 10M cells



<sup>†</sup> Wen u. a., "Dispersion of carbon dioxide from vertical vent and horizontal releases—a numerical study".

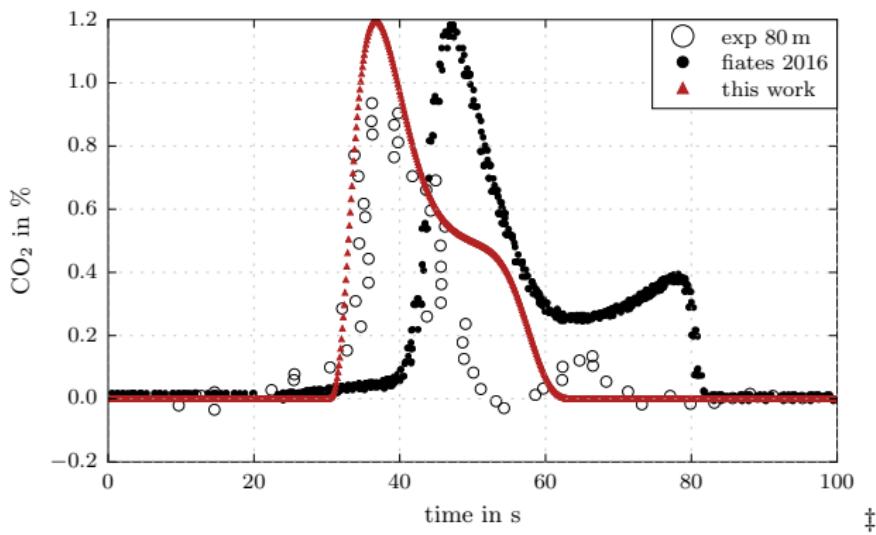


## Contour of CO<sub>2</sub> concentration=1%





## CO<sub>2</sub> concentration at 80 m

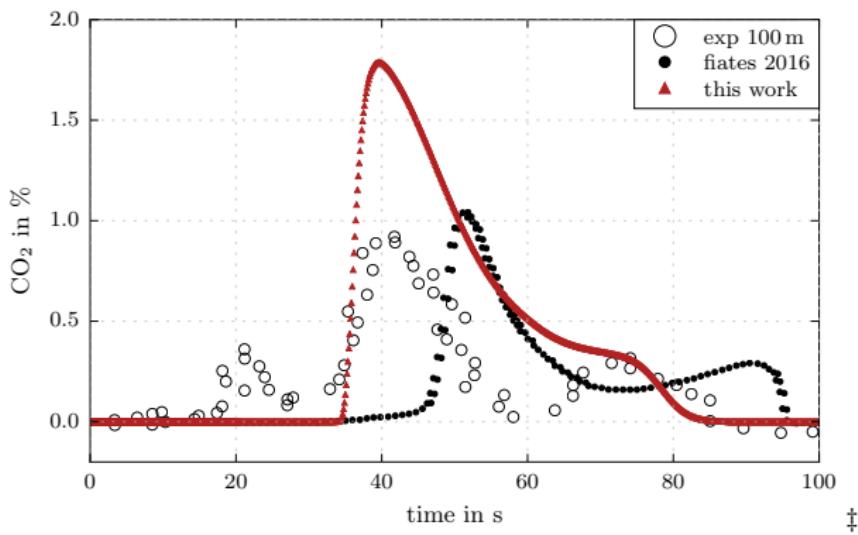


- Good agreement with measurements
- Maximum is slightly overpredicted, second peak not occurs

‡ Julianne Fiates u. a. "An alternative CFD tool for gas dispersion modelling of heavy gas". In: *Journal of Loss Prevention in the Process Industries* 44 (2016), S. 583–593.



## CO<sub>2</sub> concentration at 100 m



- Good agreement with increasing time of CO<sub>2</sub>
- Overpredicted maximum, second peak is only indicated

<sup>†</sup> Fiates u. a., "An alternative CFD tool for gas dispersion modelling of heavy gas".



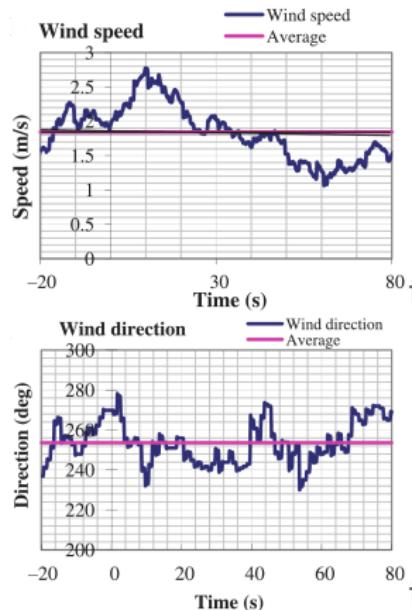
In this comparison

- Fluctuation in wind speed and direction

In general:

- Measurements in the field are not repeatable
- RANS fluctuations are completely modelled
- Modelling of highly rough walls is still subject of research

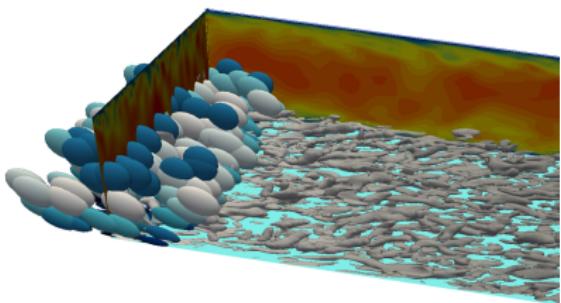
- Using high quality wind tunnel measurements for different urban environments
- Long time intervals for statistical analysis of turbulence and gas occurrence



† Wen u. a., "Dispersion of carbon dioxide from vertical vent and horizontal releases—a numerical study".



- Verify the LeMoS-Inflow-Generator for urban atmospheric boundary layer (currently working on this, using measurements of Michelstadt experiment)
  - ⇒ Reproduce urban atmospheric boundary layer with LES simulation in free terrain (wall function or porous media at the bottom, periodic BC)
  - ⇒ Verify turbulence properties
  - ⇒ Extract U-profiles, length scales L and reynolds stresses R
  - ⇒ Inflow-Generator in same domain
  - ⇒ Validate turbulent boundary layer
- Dispersion simulation with Inflow-Generator in urban environment





Thank you for your attention!