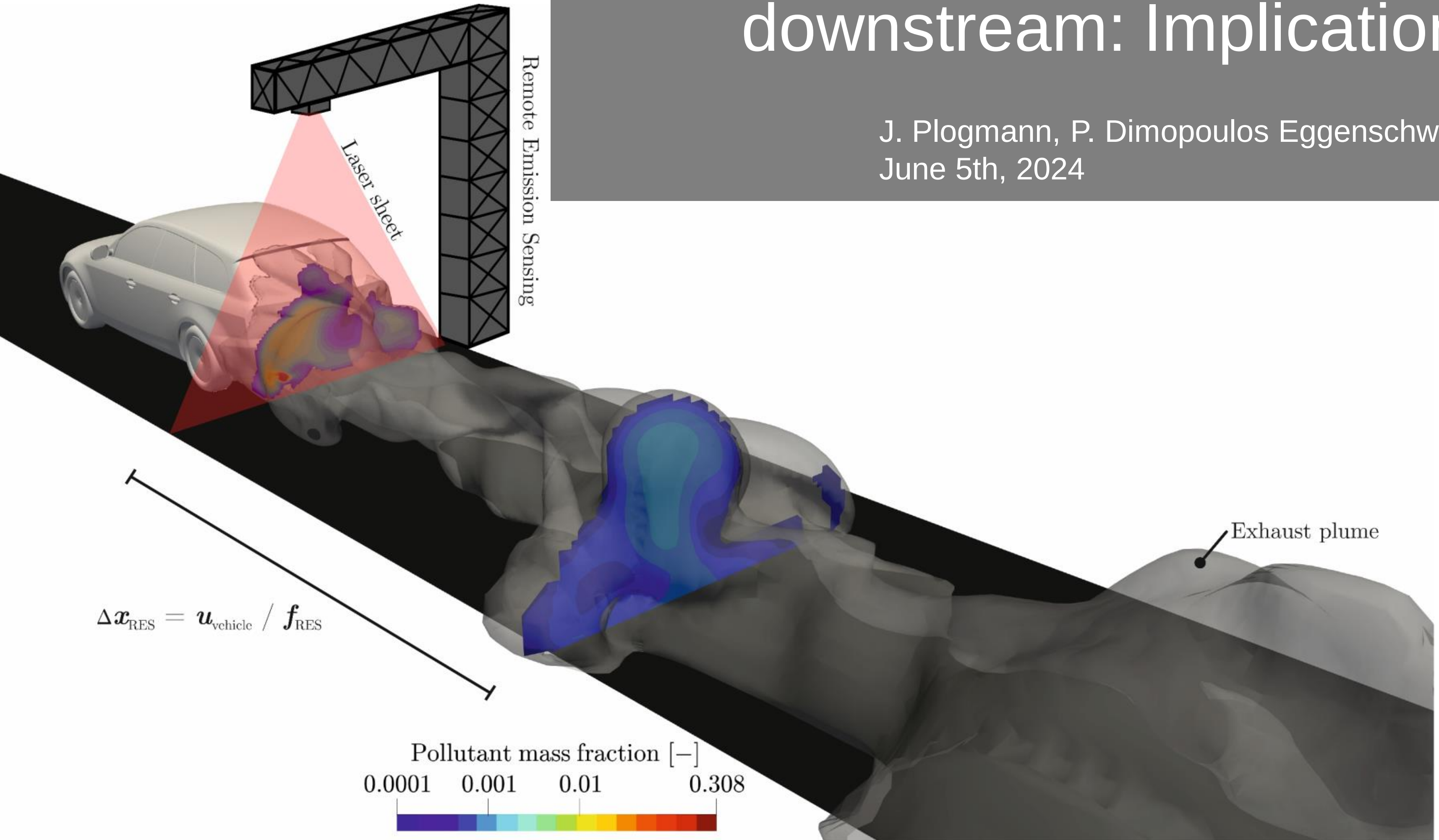
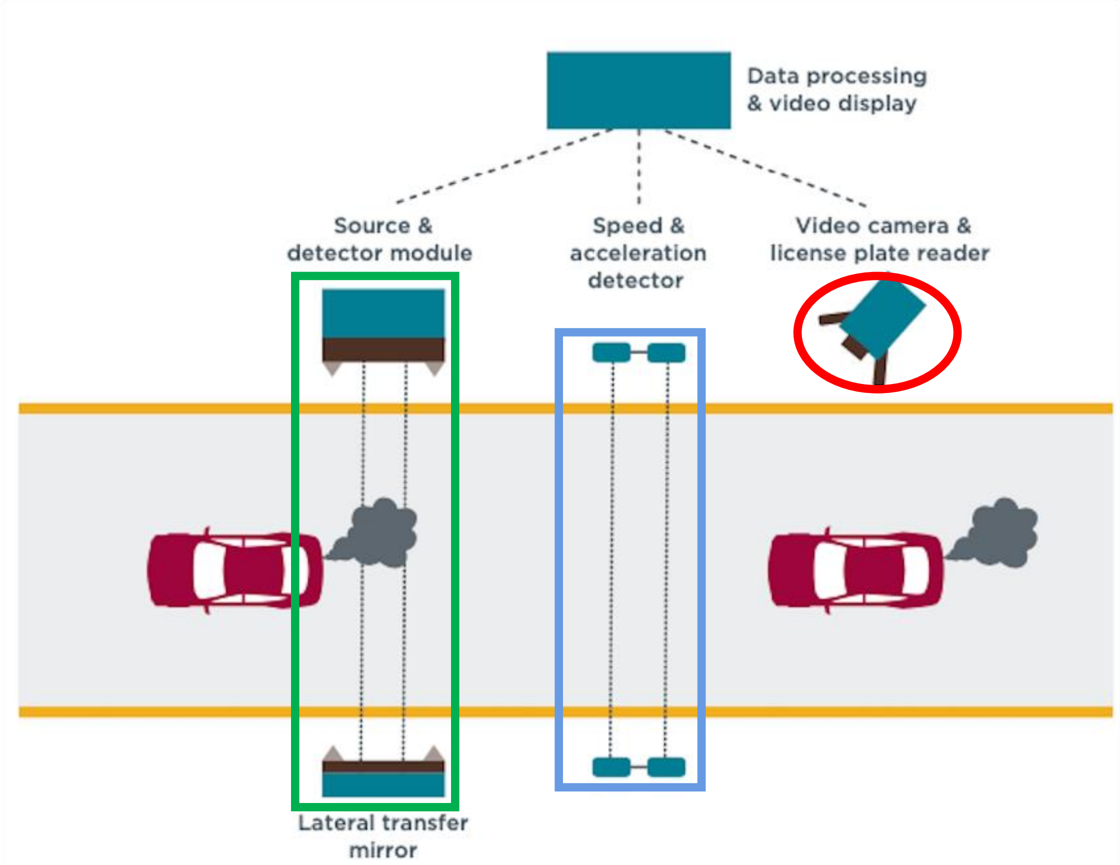
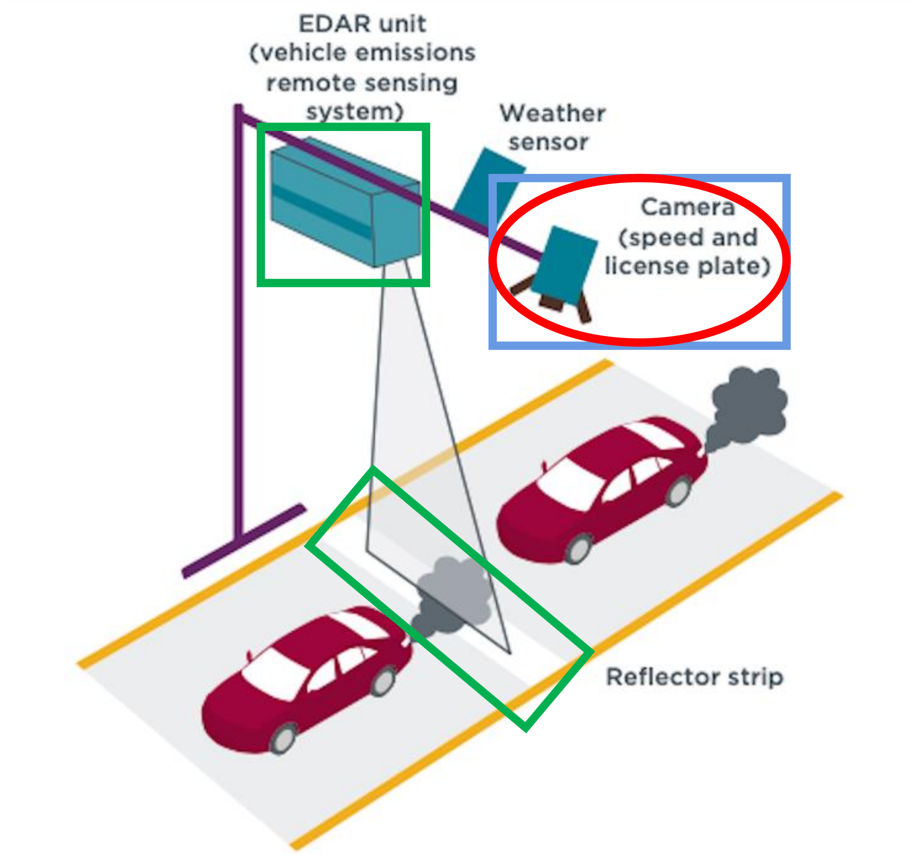
Numerical Simulation of the flow in the vehicle downstream: Implications for Remote Sensing

J. Plogmann, P. Dimopoulos Eggenschwiler
June 5th, 2024



There are two types of RES systems available





FEAT : Fuel **E**fficient **A**utomobile **T**est

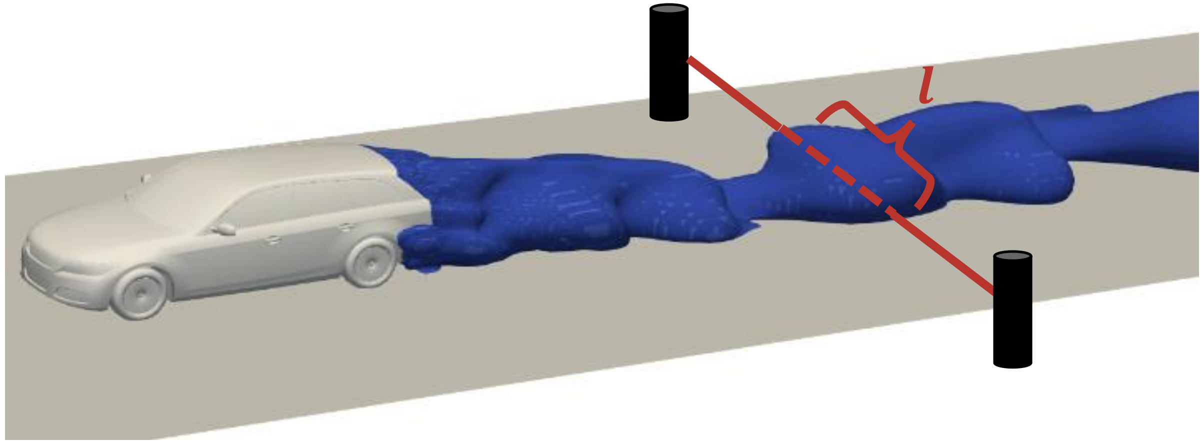
EDAR : Emission **D**etector **A**nd **R**eporting

Source: Anenberg, S., Miller, J., Minjares, R. *et al.* Impacts and mitigation of excess diesel-related NO_x emissions in 11 major vehicle markets. *Nature* **545**, 467–471 (2017). https://doi.org/10.1038/nature22086

Empa Materials Science and Technology | ivl Swedish Environmental Research Institute | Ministry of Environment of Denmark Environmental Protection Agency | VTT | ETH zürich

The result of a RES measurement is in gr pollutant per gr CO_2

Task 61



Normal substances: CO_2, H_2O, N_2, O_2

Pollutants: CO, NO, NO_2, C_2H_4 (THC)

Simulation of the exhaust plume

What is measured by the remote sensor: $\frac{\text{Pollutants}}{\text{Fuel consumption}} \propto \frac{c_{NO_x}}{c_{CO_2}}$

Relation calibrated in laboratory: Voltage $\propto \frac{1}{A_\lambda}$

Beer-Lambert law: $A_\lambda = \epsilon_\lambda \cdot c \cdot l$

$$c = \frac{A_\lambda}{\epsilon_\lambda \cdot l}$$

- A Optical attenuation
- ϵ Molar attenuation coefficient (adsorptivity)
- c Concentration of species
- l Optical path length

Empa Materials Science and Technology

Ministry of Environment of Denmark Environmental Protection Agency

Research Institute

Focus: Simulations and specific evaluations of measurement data

- WP 1: Numerical Simulation of the dispersion of a pollutant in the vehicle
- WP2: Relation of RES measured data to the actual vehicle emission
- WP 3: Potential of RES measurements for determining aging of vehicles' exhaust aftertreatment systems in the field
- WP 4: Technical exchange with the other countries in the project, other projects. Integration of the Swiss measurements in the CONOx database

Empa Materials Science and Technology | ivl Swedish Environmental Research Institute | Ministry of Environment of Denmark Environmental Protection Agency | VTT | ETH zürich

Focus: Simulations and specific evaluations of measurement data

- WP 1: Numerical Simulation of the dispersion of a pollutant in the vehicle
- WP2: Relation of RES measured data to the actual vehicle emission
- WP 3: Potential of RES measurements for determining aging of vehicles' exhaust aftertreatment systems in the field
- WP 4: Technical exchange with the other countries in the project, other projects. Integration of the Swiss measurements in the CONOx database

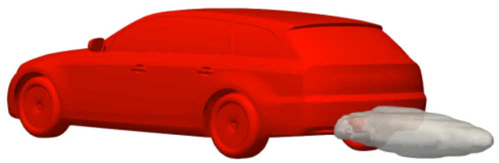
Empa Materials Science and Technology
ivl Swedish Environmental Research Institute
Ministry of Environment of Denmark Environmental Protection Agency
VTT
ETH zürich

Flow in the vehicle wake: unsteady, turbulent, heat and species transport

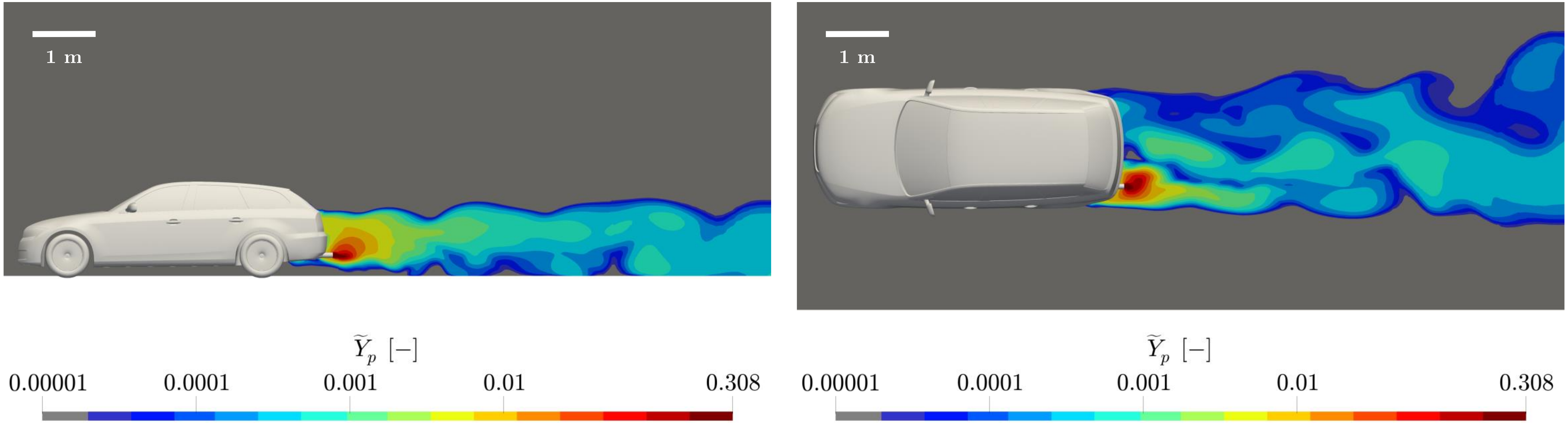
URANS

$v_{\text{vehicle}} = 50$ km/h

$Re_L = 4{,}257{,}166$



Pollutant concentrations decay rapidly in the vehicle wake

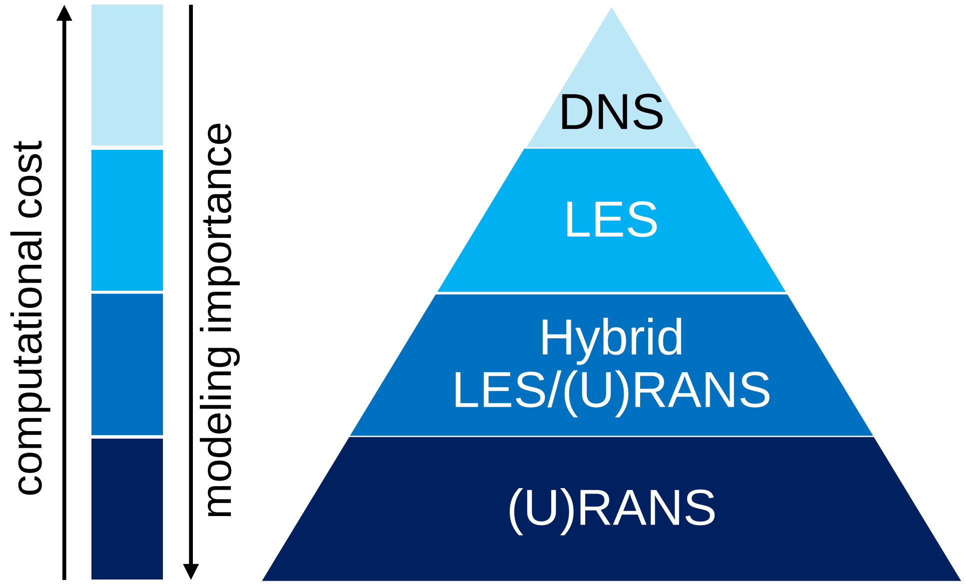


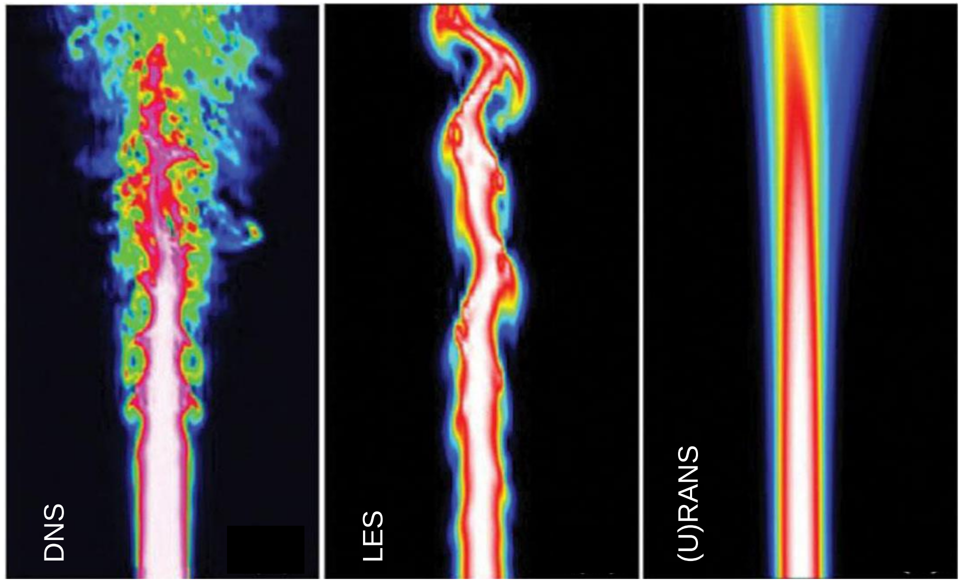
Source: Plogmann, J.; Stauffer, C.; Dimopoulos Eggenschwiler, P.; Jenny, P. URANS Simulations of Vehicle Exhaust Plumes with Insight on Remote Emission Sensing. *Atmosphere* **2023**, *14*, 558. https://doi.org/10.3390/atmos14030558

- Turbulent dispersion is dominant: $D_{\mathrm{eff}} = D + D_t$ with $D_t \gg D$
- Thus, the modeling of D_t plays a crucial role for an accurate prediction of the plume dispersion

Turbulence is nowadays one of the most important unsolved problems in physics

Task 61





- The computational cost of DNS and LES is dependent on the Reynolds number: $Re = (u_{\infty}L)/\nu$
  - DNS scales with Re^{3}
  - LES scales with $Re^{1.8}$ near the wall and $Re^{0.4}$ in the free-shear region
- (U)RANS only provides information about averaged quantities but at low computational cost

Empa Materials Science and Technology
ivl Swedish Environmental Research Institute
Ministry of Environment of Denmark Environmental Protection Agency
VTT
ETH zürich

Reynolds-Averaged Navier-Stokes-Fourier system of equations (URANS)

N.S.F. equations → Ensemble-Averaging $\tilde{\phi} = \frac{\overline{\rho\phi}}{\bar{\rho}}$ → k-ω SST model

PISO Algorithm
Finite Volume Method

Momentum equation:

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial\left(\bar{p} + \frac{2}{3}\bar{\rho}k\right)}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu_{\text{eff}}\left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial\tilde{u}_k}{\partial x_k}\delta_{ij}\right)\right] + \bar{\rho}\tilde{g}_i$$

Total energy equation:

$$\frac{\partial}{\partial t}\left[\bar{\rho}\left(\tilde{e} + \frac{1}{2}\tilde{u}_i\tilde{u}_i + K\right)\right] + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{u}_j\left(\tilde{h} + \frac{1}{2}\tilde{u}_i\tilde{u}_i + K\right)\right] = \frac{\partial}{\partial x_j}\left(\alpha_{\text{eff}}\frac{\partial\tilde{h}}{\partial x_j}\right) + \bar{\rho}\tilde{g}_i\tilde{u}_i$$

Species equation:

$$\frac{\partial(\bar{\rho}\widetilde{Y_k})}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\widetilde{Y_k}) = \frac{\partial}{\partial x_i}\left(\bar{\rho}D_{\text{eff}}\frac{\partial\widetilde{Y_k}}{\partial x_i}\right)$$

Equation of state (ideal gas):

$$\bar{p} = \bar{\rho}R\tilde{T}\sum_k^n\frac{\widetilde{Y_k}}{W_k}$$

Sutherland law:

$$\mu = \frac{A_s\sqrt{\tilde{T}}}{1 + T_s/\tilde{T}}$$

Schmidt law:

$$Sc = \frac{\mu}{\bar{\rho}D} = 1$$

$$Sc_t = \frac{\mu_t}{\bar{\rho}D_t} = 0.7$$

Prandtl law:

$$Pr = \frac{\mu}{\bar{\rho}\alpha} = 0.9$$

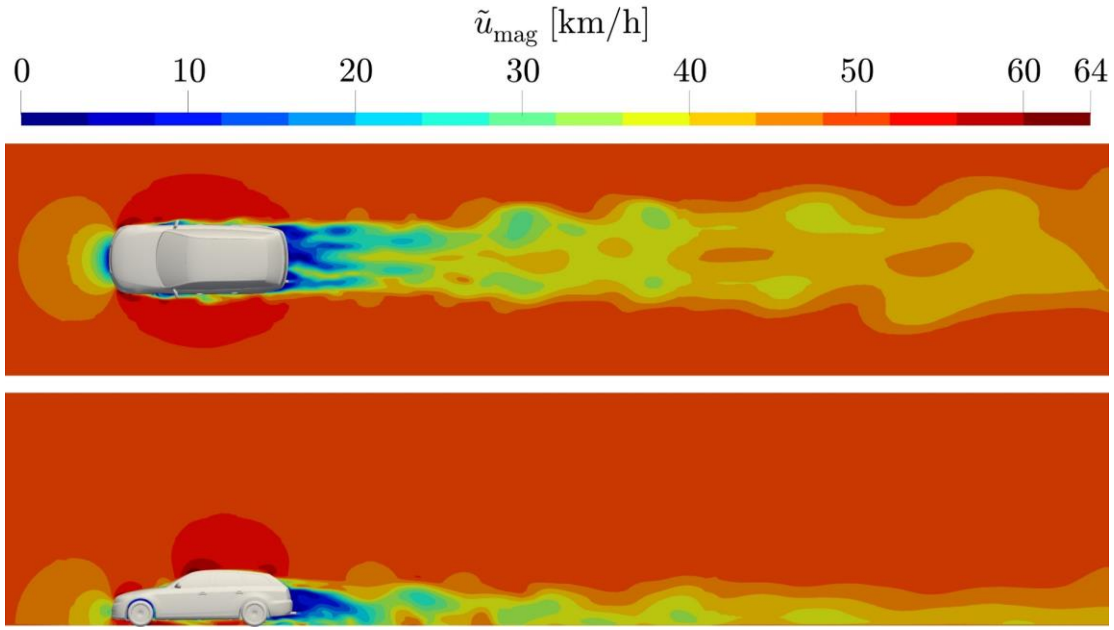
$$Pr_t = \frac{\mu_t}{\bar{\rho}\alpha_t} = 0.9$$

JANAF tables:

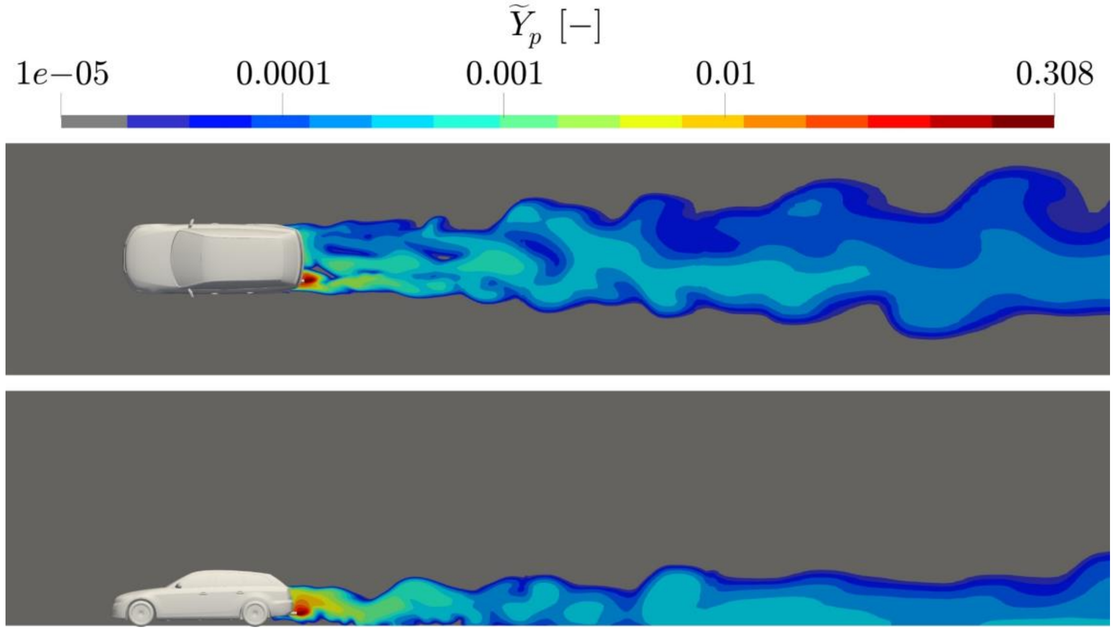
c_p , c_v

Unsteady and turbulent flow yields time-dependent velocity and pollutant fields

Task 61



Instantaneous velocity magnitude at $z = 0.3$ m plane (top) and $y = -0.56$ m plane (bottom).



Instantaneous pollutant mass fraction at $z = 0.3$ m plane (top) and $y = -0.56$ m plane (bottom).

Empa Materials Science and Technology

ivl Swedish Environmental Research Institute

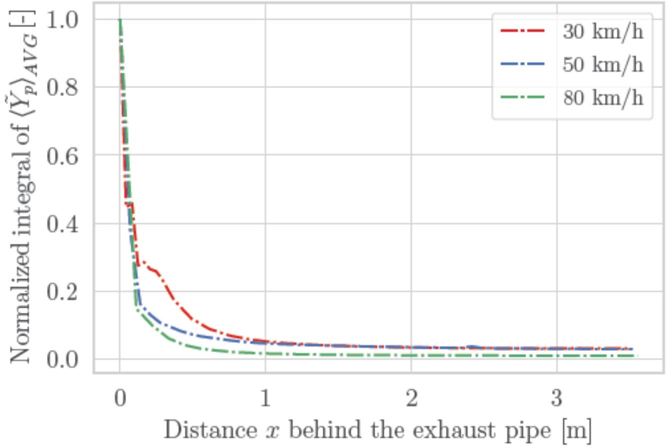
Ministry of Environment of Denmark Environmental Protection Agency

VTT

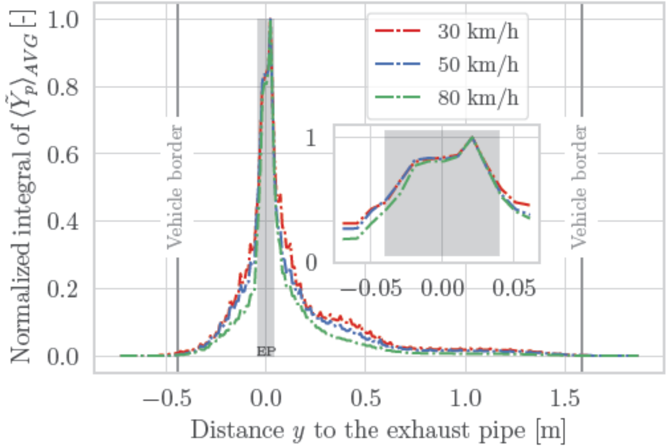
ETH zürich

Vehicle speed influences the exhaust plume dispersion in all directions

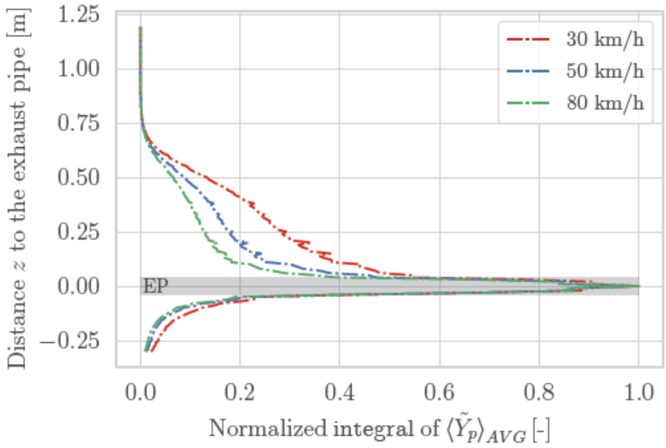
Task 61



(a) Normalized cut plane integral of time-averaged pollutant mass fraction in the yz-planes.



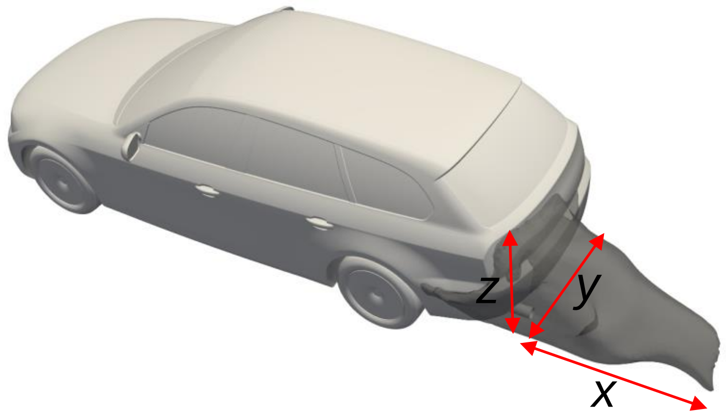
(b) Normalized cut plane integral of time-averaged pollutant mass fraction in the xz-planes.



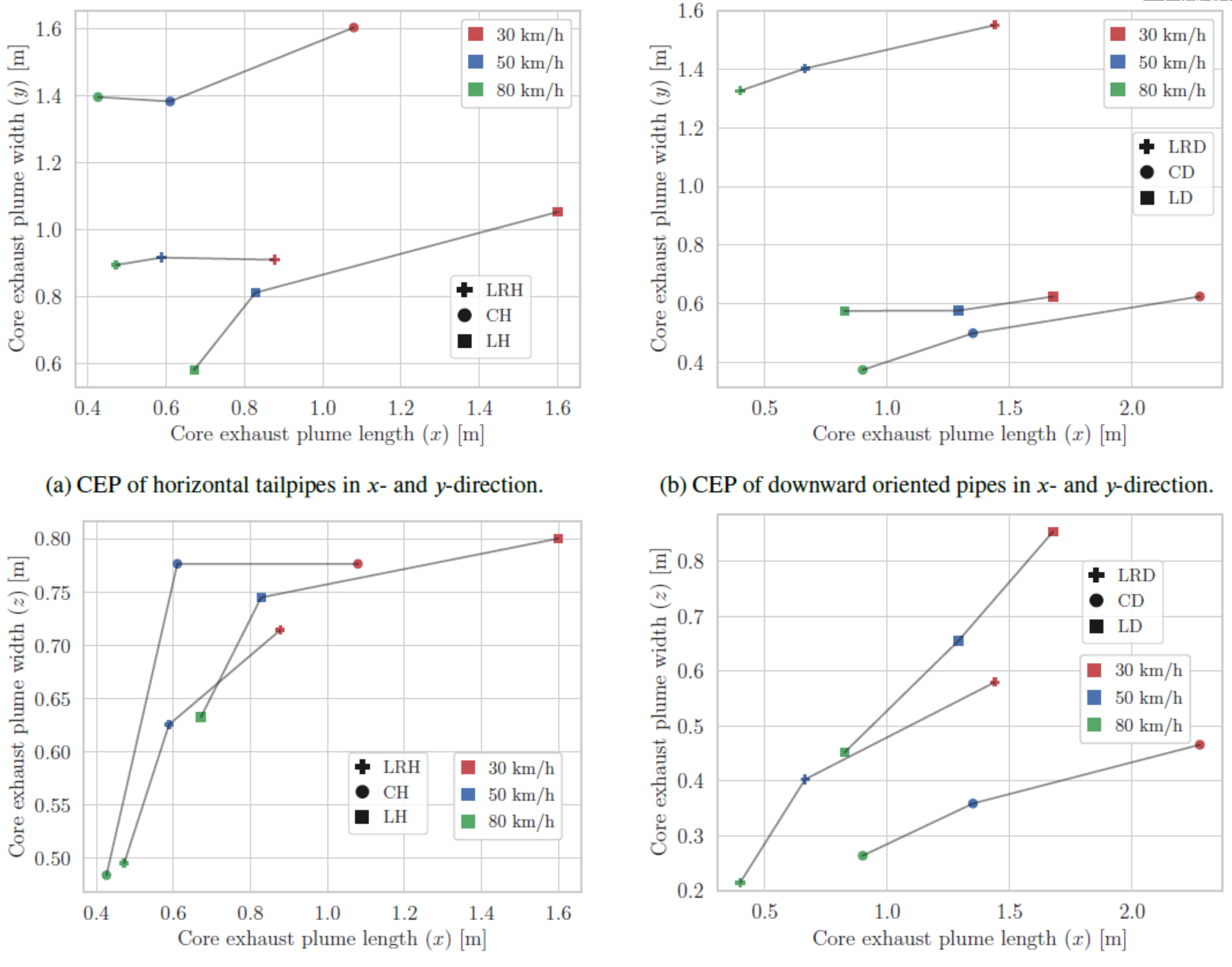
(c) Normalized cut plane integral of time-averaged pollutant mass fraction in the xy-planes.

Pollutant dispersion behavior of a vehicle at 30,50 and 80 km/h.

With increasing vehicle speed, the (Core) Exhaust Plume (CEP) gets shorter



CEP is the plume up to a hundredfold dilution of the initial exhaust tailpipe concentration



(a) CEP of horizontal tailpipes in x- and y-direction.

(b) CEP of downward oriented pipes in x- and y-direction.

(c) CEP of horizontal tailpipes in x- and z-direction.

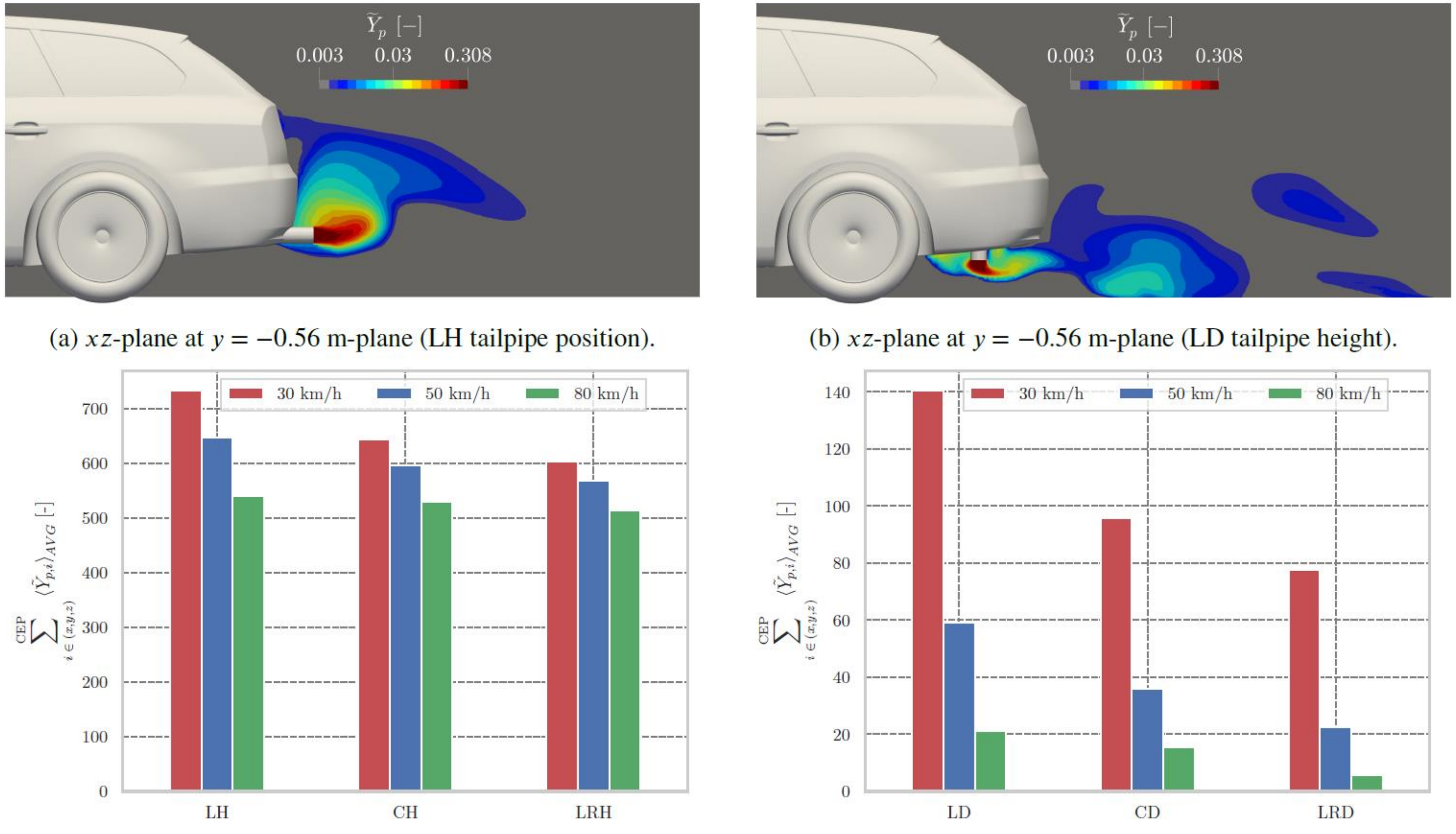
(d) CEP of downward oriented pipes in x- and z-direction.

Empa Materials Science and Technology

ivl Swedish Environmental Research Institute

Protection Agency

Different pipe positions change the amount of pollutant in core exhaust plume



(a) xz-plane at $y = -0.56$ m-plane (LH tailpipe position).

(b) xz-plane at $y = -0.56$ m-plane (LD tailpipe height).

(c) Tailpipe locations are LH, CH and LRH.

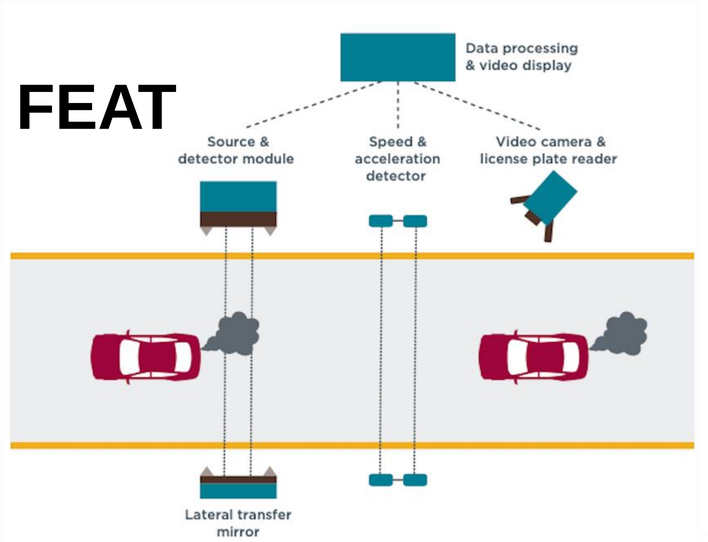
(d) Tailpipe locations are LD, CD and LRD.

Sum of all time-averaged pollutant at x,y and z in the core exhaust plume (CEP) in case of 30, 50 and 80 km/h vehicle speed. Tailpipe locations are left horizontally oriented (LH), central horizontally oriented (CH) as well as left and right horizontally oriented (LRH).

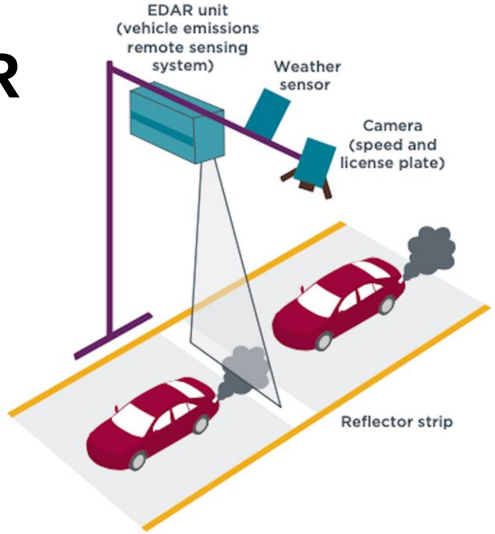
Materials Science and Technology
Research Institute
Protection Agency

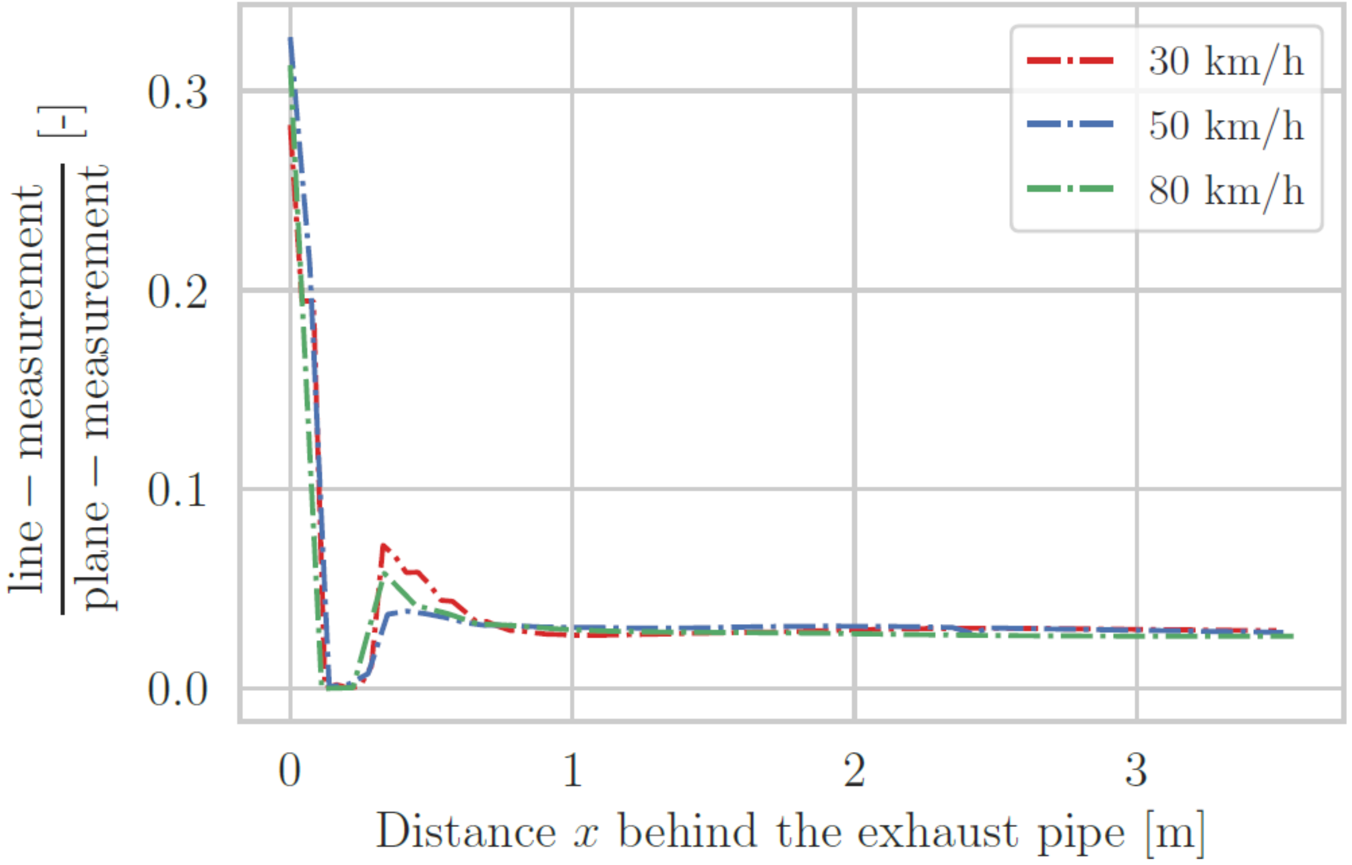
The light beam instrument can capture max. 30% of the plume captured by a laser sheet instrument

FEAT



EDAR



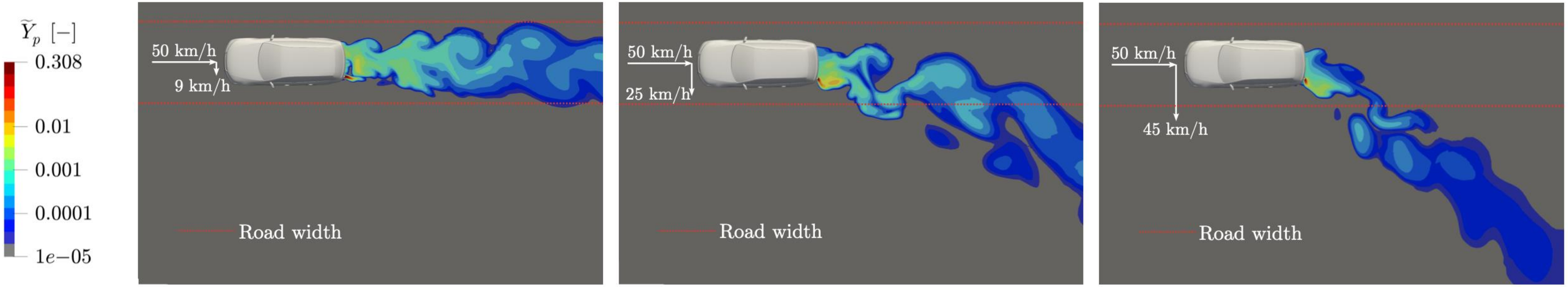


Ratio of the sum of time-averaged pollutant mass fraction of FEAT (line in y-direction at tailpipe height $z = 0.3$ m) and EDAR (yz-plane).

Environmental Protection Agency

Increasing crosswind speed causes stronger deflection and oscillations of the exhaust plume

Task 61



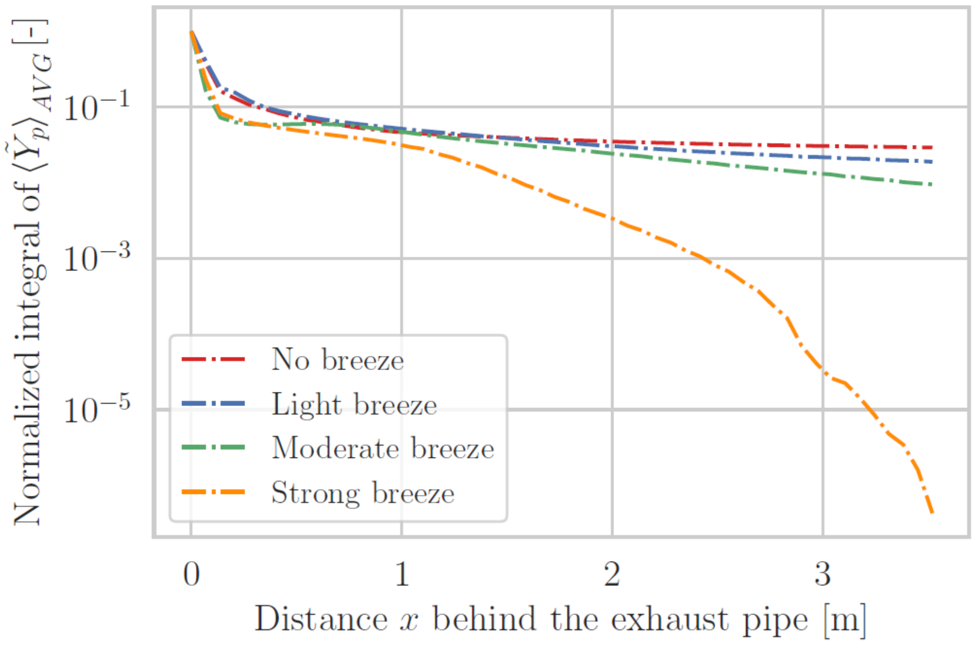
(a) Light breeze. (b) Moderate breeze. (c) Strong breeze.

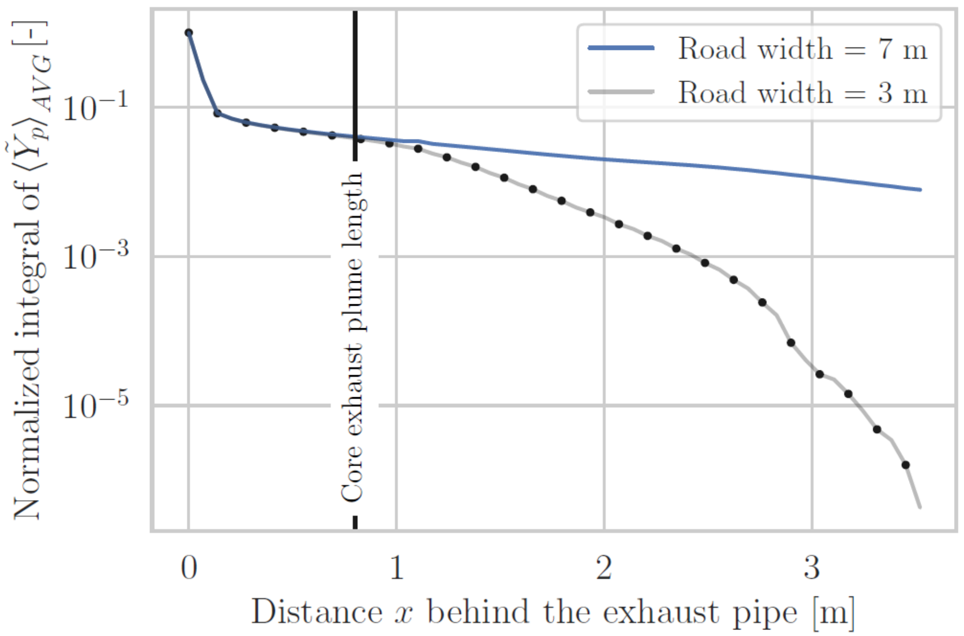
Exhaust plume deflection under influence of light, moderate and strong breeze from the right side (90°) in case of a vehicle driven at 50 km/h with a horizontally oriented tailpipe on the left. Planes are extracted for a road width of 3 m.

Empa Materials Science and Technology · ivl Swedish Environmental Research Institute · Ministry of Environment of Denmark Environmental Protection Agency · VTT · ETH zürich

Core exhaust plume deflection is rather small

Task 61



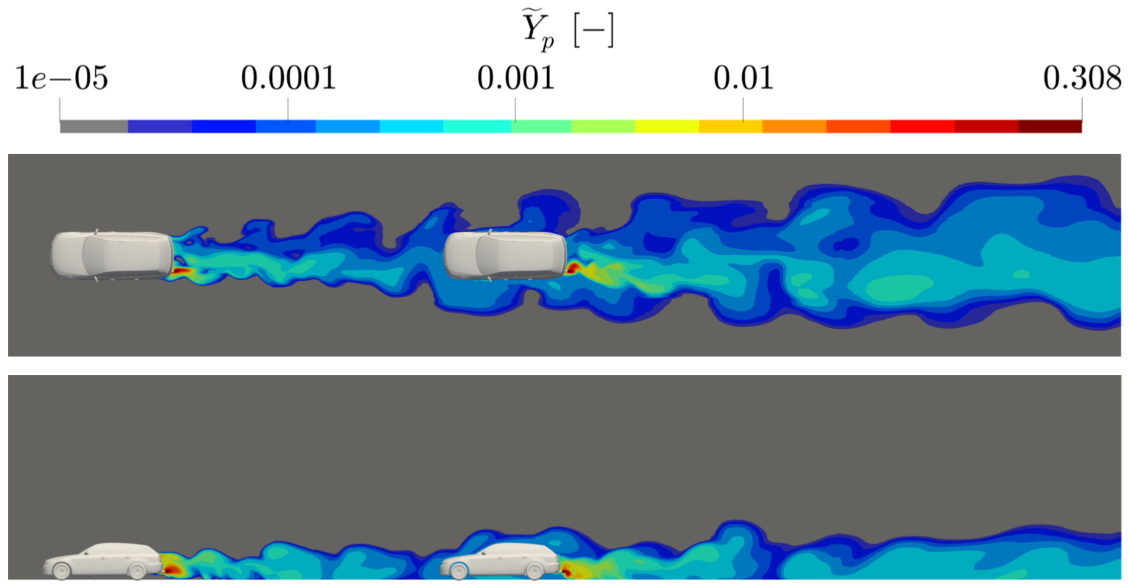


Integral of time-averaged pollutant mass fraction in yz-plane under influence of light, moderate and strong breeze coming from the right side (90°). The vehicle is driving at 50 km/h and has a horizontally oriented tailpipe on the left. Road width is 3 m.

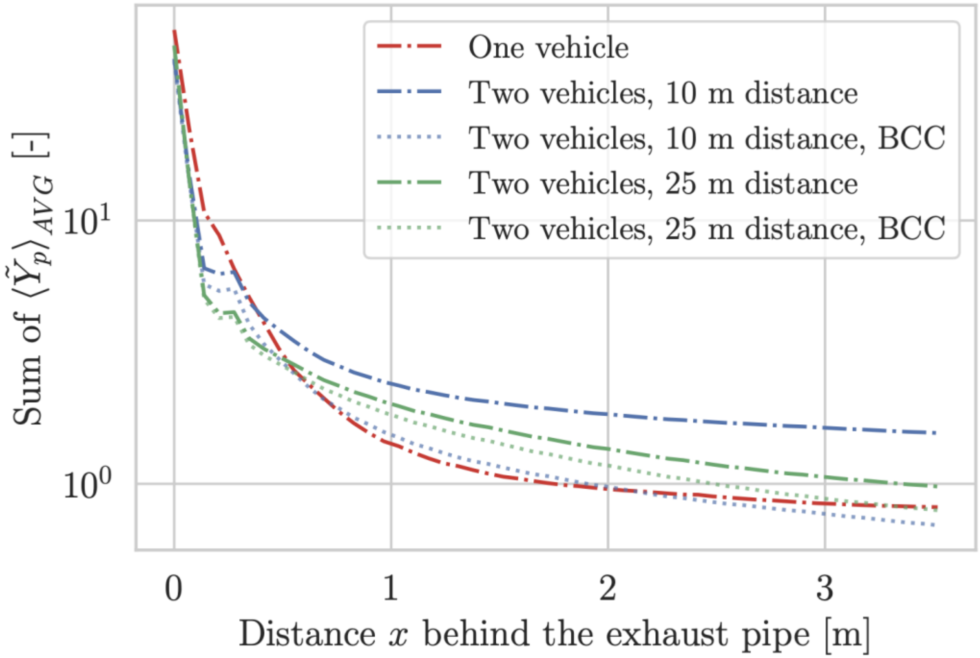
Influence of road width in case of a vehicle driving at 50 km/h with a horizontally oriented tailpipe on the left side, where crosswind is acting from the side (90°) at 45 km/h.

Empa Materials Science and Technology
ivl Swedish Environmental Research Institute
Ministry of Environment of Denmark Environmental Protection Agency
VTT
ETH zürich

Vehicle ahead causes more chaotic flow in front of the following vehicle. “Background” concentration from vehicle ahead (after 10 and 25 m) is negligible



Pollutant mass fraction at $z = 0.3$ m plane (top) and $y = -0.57$ m plane (bottom) of two vehicles driving at 50 km/h 10 m apart from the other, both with horizontally oriented pipes on the left side.

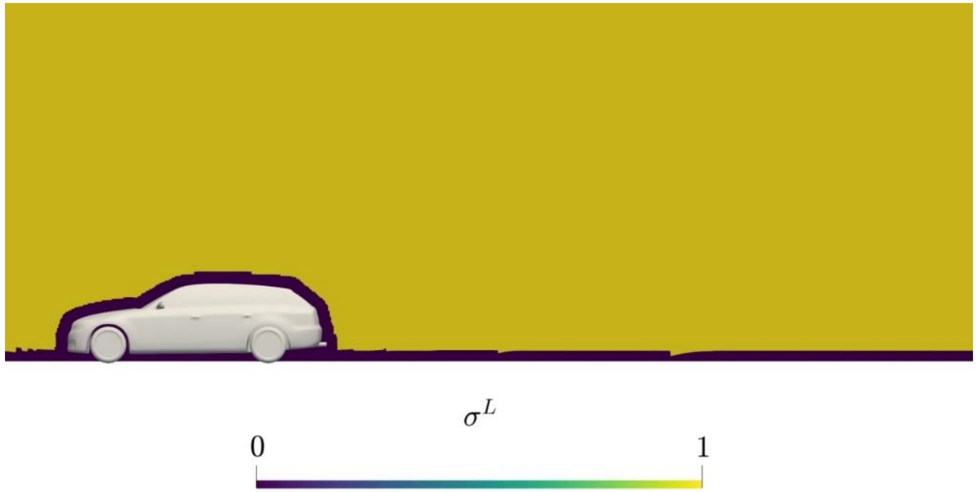


Empa
Materials Science and Technology

ivl
Swedish Environmental Research Institute

Ministry of Enviro
of Denmark
Environmental Protection Agency

Consistent hybrid LES/RANS dual-mesh framework



RANS:

$$\frac{\partial \langle\rho\rangle \widehat{u}_i}{\partial t} + \frac{\partial \langle\rho\rangle \widehat{u}_i \widehat{u}_j}{\partial x_j} = -\frac{\partial \langle p\rangle}{\partial x_i} + \frac{\partial}{\partial x_j} 2\langle\rho\rangle \left[(\nu+\nu_t)\widehat{S}_{ij} - \frac{1}{3}\delta_{ij}\left(\nu \frac{\partial \langle u_k\rangle}{\partial x_k} + k\right)\right] + \langle\rho\rangle \boxed{Q^R_{u,i}}$$

LES:

$$\frac{\partial \langle\rho\rangle \widehat{u}_i}{\partial t} + \frac{\partial \langle\rho\rangle \widehat{u}_i \widehat{u}_j}{\partial x_j} = -\frac{\partial \langle p\rangle}{\partial x_i} + \frac{\partial \left(\langle\tau^v_{ij}\rangle - \langle\rho\rangle \widehat{u''_i u''_j}\right)}{\partial x_j} + \langle\rho\rangle \boxed{Q^R_{u,i}}$$

Drift term:

$$Q^R_{u,i} = \begin{cases} \frac{\langle\overline{u}_i\rangle^{AVG} - \langle u_i\rangle}{\gamma_r} & \text{in LES regions and} \\ 0 & \text{in RANS regions.} \end{cases}$$

Averaging:

$$\langle\phi\rangle^{AVG,n} = (1-\alpha)\phi^n + \alpha\langle\phi\rangle^{AVG,n-1}$$

$$\text{with } \alpha = \frac{1}{1+\Delta t/T}$$

Consistency:

$$\langle\overline{u}_i\rangle^{AVG} \approx \langle u_i\rangle$$
$$\langle\tau_{ij}\rangle^{AVG} \approx \langle u'_i u'_j\rangle$$
$$\langle\varepsilon\rangle^{AVG} \approx \varepsilon^R$$

Drift term:

$$Q^L_{u,i} = \begin{cases} Q^{L,u}_i + Q^{L,g}_i & \text{in RANS regions and} \\ 0 & \text{in LES regions,} \end{cases}$$

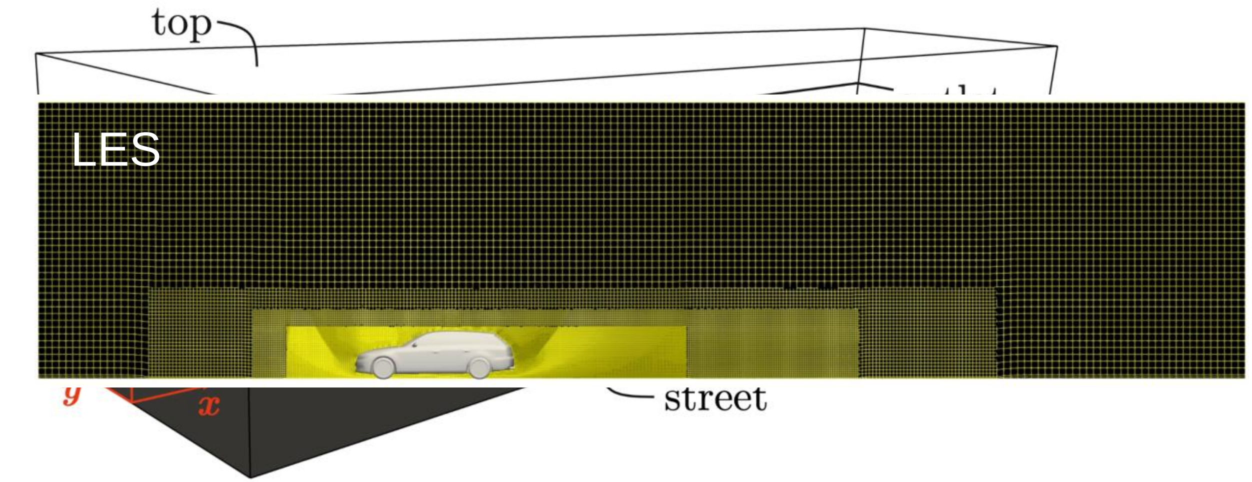
$$Q^{L,u}_i = \frac{\langle u_i\rangle - \langle\overline{u}_i\rangle^{AVG}}{\gamma_l}$$

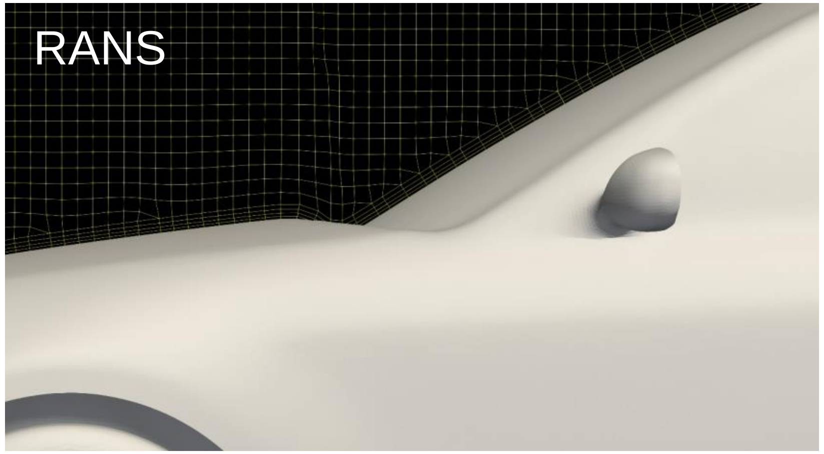
$$Q^{L,g}_i = G_{ij}\frac{\langle\overline{u}_j\rangle^{AVG} - \overline{u}_j}{\gamma_g}$$

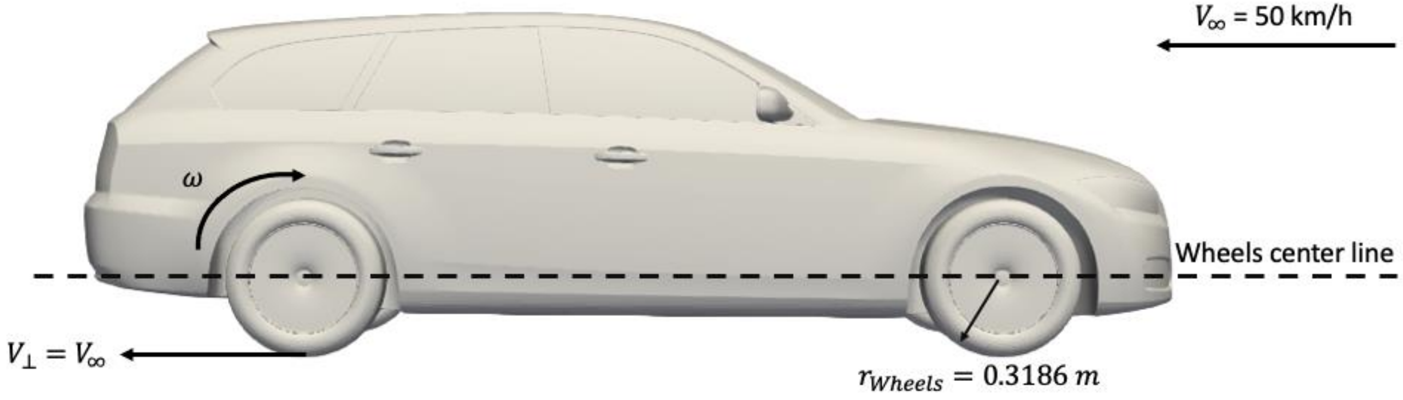
$$G_{ij} = \frac{\langle\tau_{ij}\rangle^{AVG} - \langle u'_i u'_j\rangle}{\langle\tau_{kk}\rangle^{AVG} + \langle u'_k u'_k\rangle}$$

Materials Science and Technology
Swedish Environmental Research Institute
of Denmark Environmental Protection Agency
zurich

Computational domain and dual-mesh







Car model: DrivAer

Mesh:

RANS: 2,031,997 cells

LES: 3,393,543 cells

Software: OpenFOAM

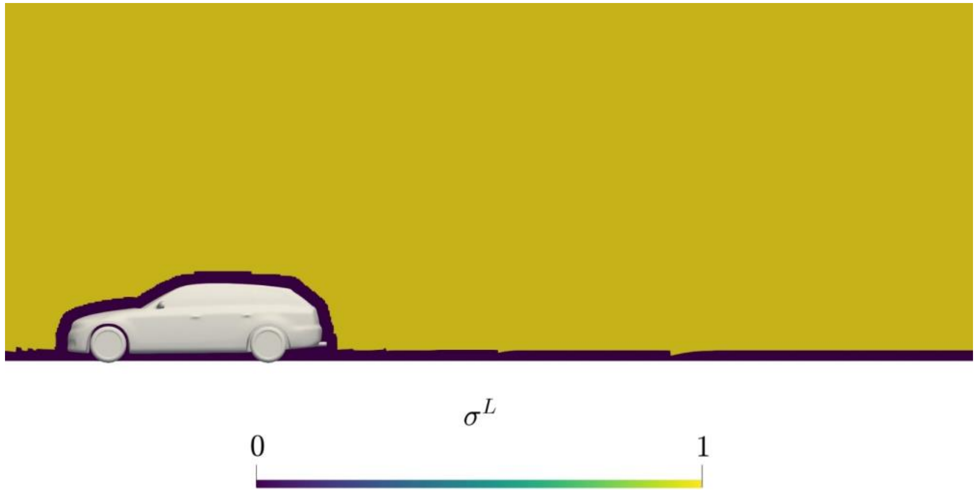
Materials Science and Technology

Swedish Environmental Research Institute

Environmental Protection Agency

Extension for scalar transport; one of the main novelties of Plogmann PhD

Task 61



RANS:

$$\frac{\partial \langle\rho\rangle \widehat{Z}}{\partial t} + \frac{\partial \langle\rho\rangle \widehat{u}_i \widehat{Z}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\langle\rho\rangle\left(\Gamma + \Gamma_t\right)\frac{\partial \widehat{Z}}{\partial x_i}\right] + \boxed{\langle\rho\rangle Q_z^R}$$

LES:

$$\frac{\partial \overline{\rho}\widetilde{Z}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i \widetilde{Z}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\overline{\rho}\left(\Gamma + \Gamma_{sgs}\right)\frac{\partial \widetilde{Z}}{\partial x_i}\right] + \boxed{\overline{\rho} Q_z^L}$$

Drift term:

$$Q_z^R = \begin{cases} \frac{\langle\widetilde{Z}\rangle^{AVG} - \hat{Z}}{\gamma_{zr}} & \text{in LES regions,} \\ 0 & \text{in RANS regions,} \end{cases}$$

Drift term:

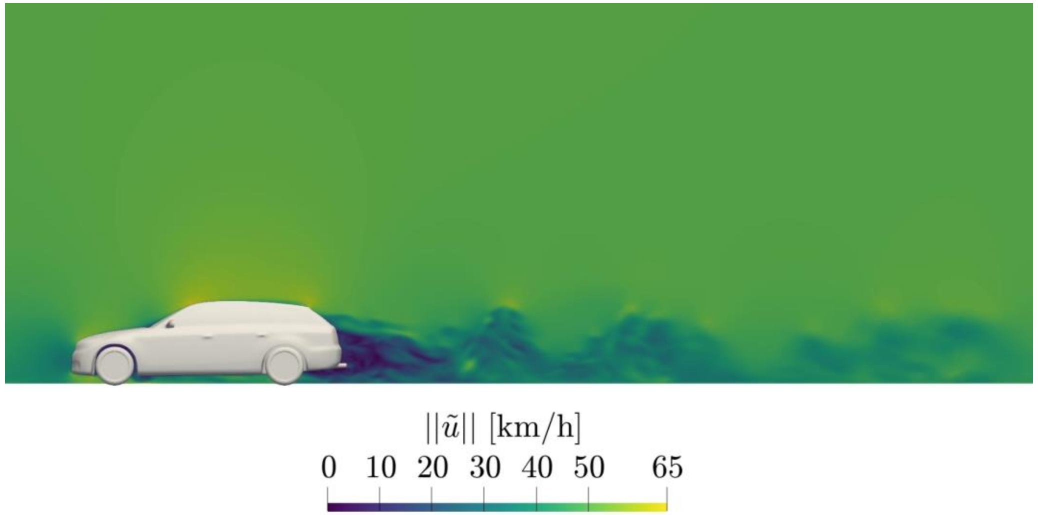
$$Q_z^L = \begin{cases} Q^{L,z} + Q^{L,\zeta} & \text{in RANS regions,} \\ 0 & \text{in LES regions,} \end{cases}$$

$$Q^{L,z} = \frac{\widehat{Z} - \langle\widetilde{Z}\rangle^{AVG}}{\gamma_{zl}}$$

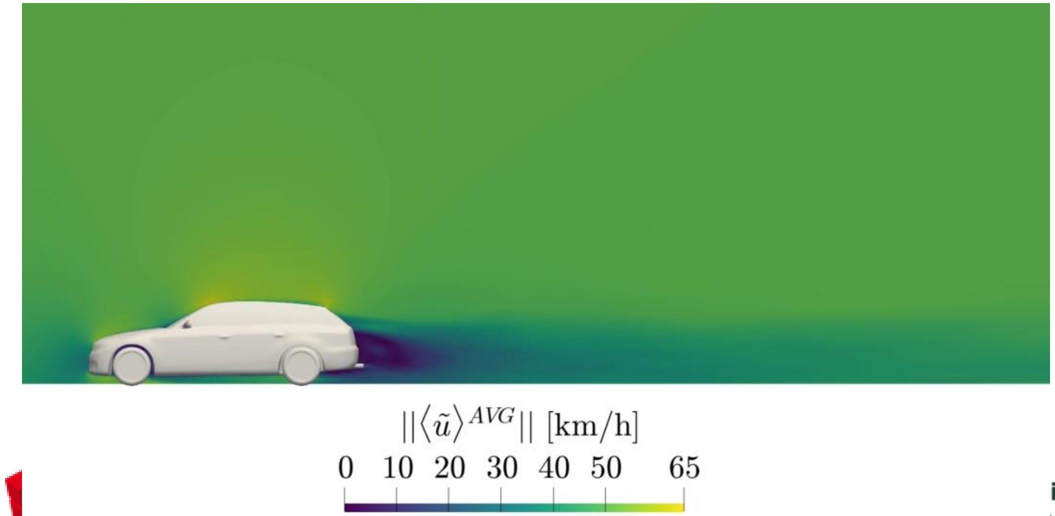
$$Q^{L,\zeta} = \left(1 - \frac{\zeta_{sgs}^{AVG}}{\zeta^{AVG}}\right)\frac{\zeta^R - \zeta^{AVG}}{\zeta^R + \zeta^{AVG}}\frac{\widetilde{Z} - \langle\widetilde{Z}\rangle^{AVG}}{2\gamma_{vl}}$$

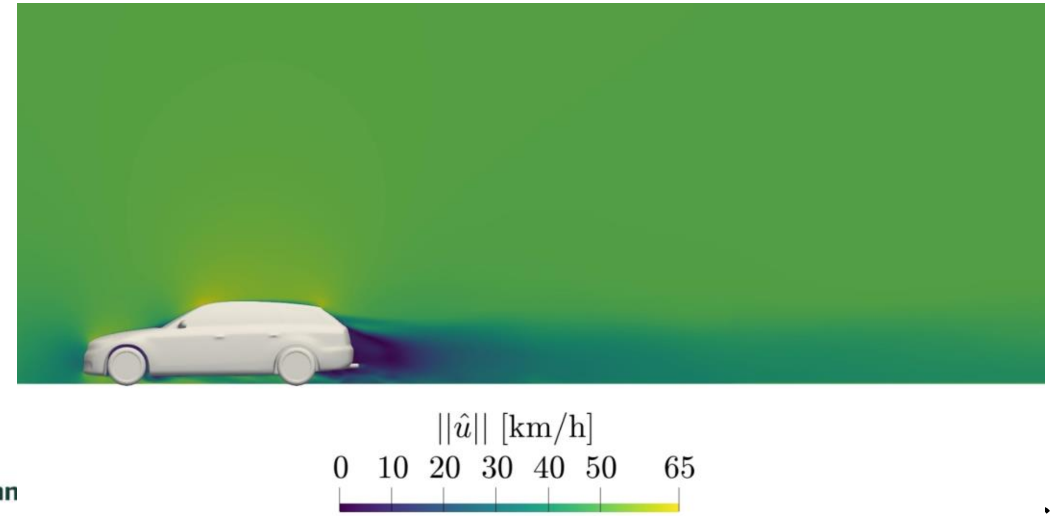
The averaged LES fields should be close to the URANS fields: Flow velocities

Task 61

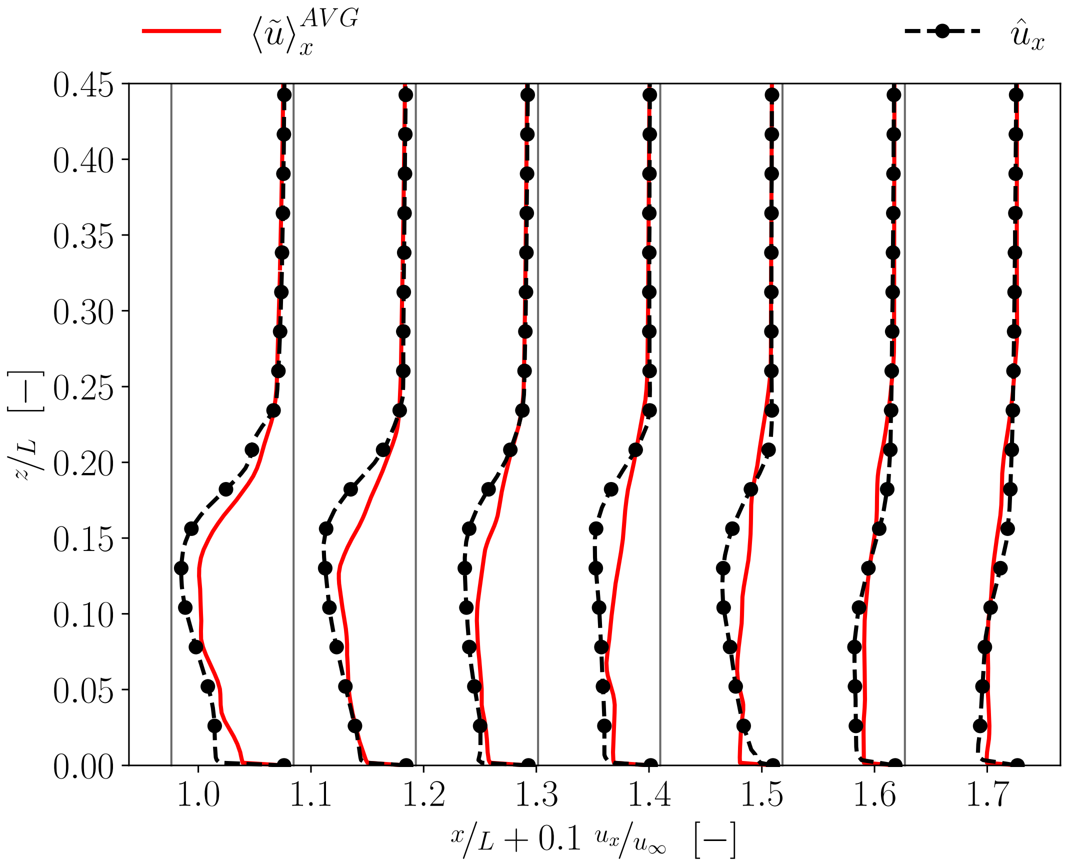


- LES provides an unsteady velocity field with fluctuations
- URANS provides an unsteady but mean velocity field without fluctuations
- Consistency is achieved between averaged LES and URANS velocities

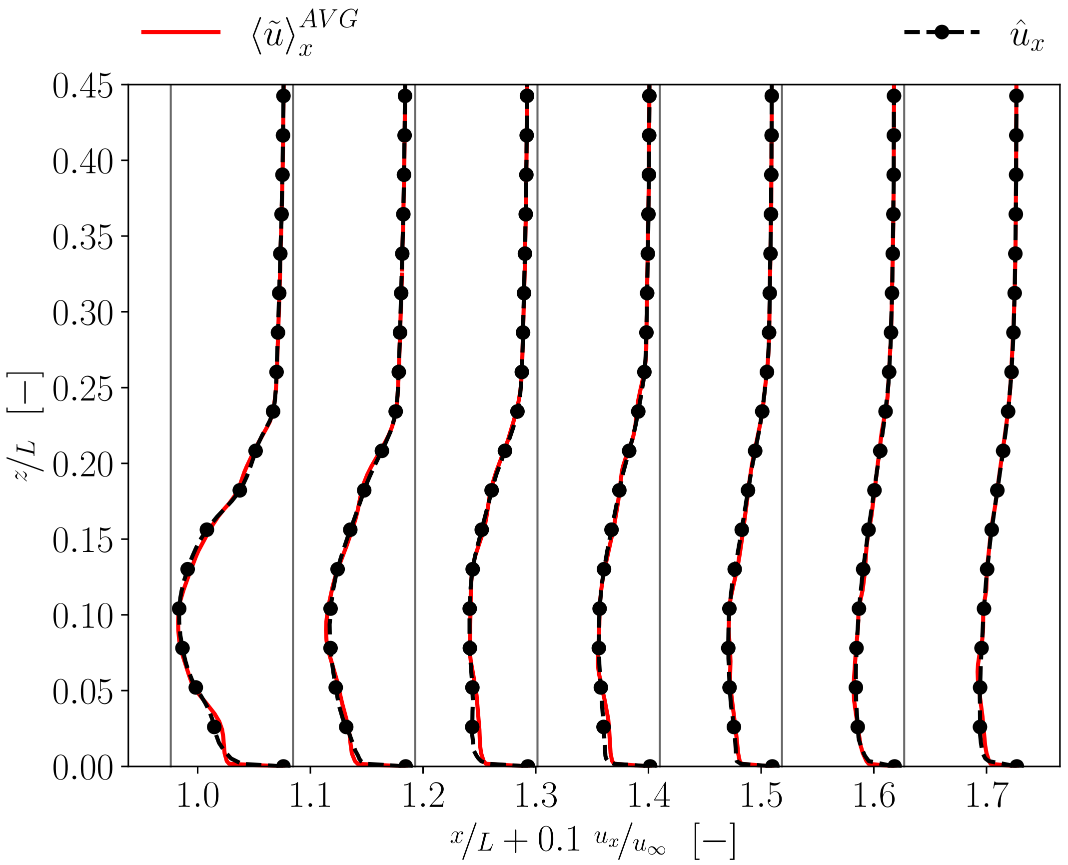




Consistency of velocity fields



Before coupling (standalone simulations)



After coupling (hybrid simulation)

Empa Materials Science and Technology

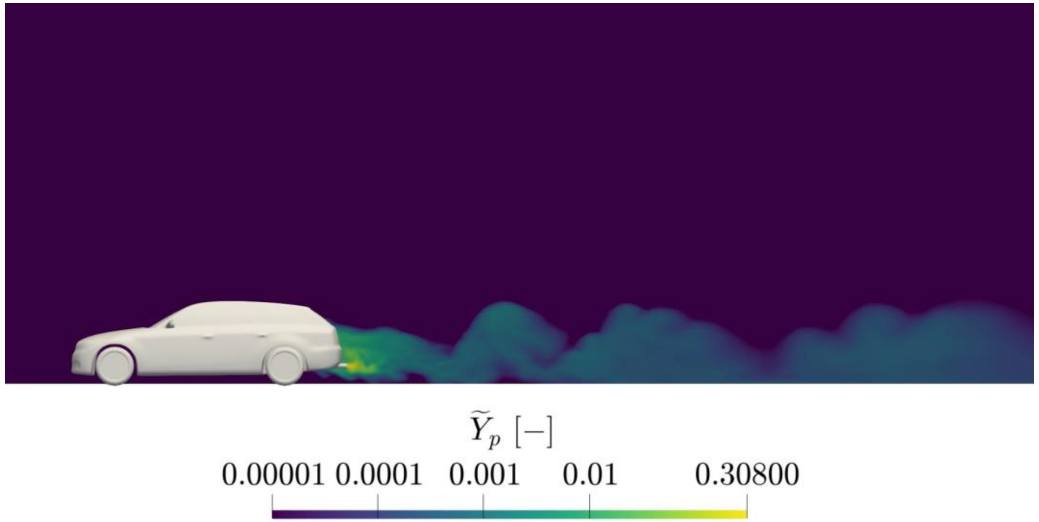
ivl Swedish Environmental Research Institute

Ministry of Environment of Denmark Environmental Protection Agency

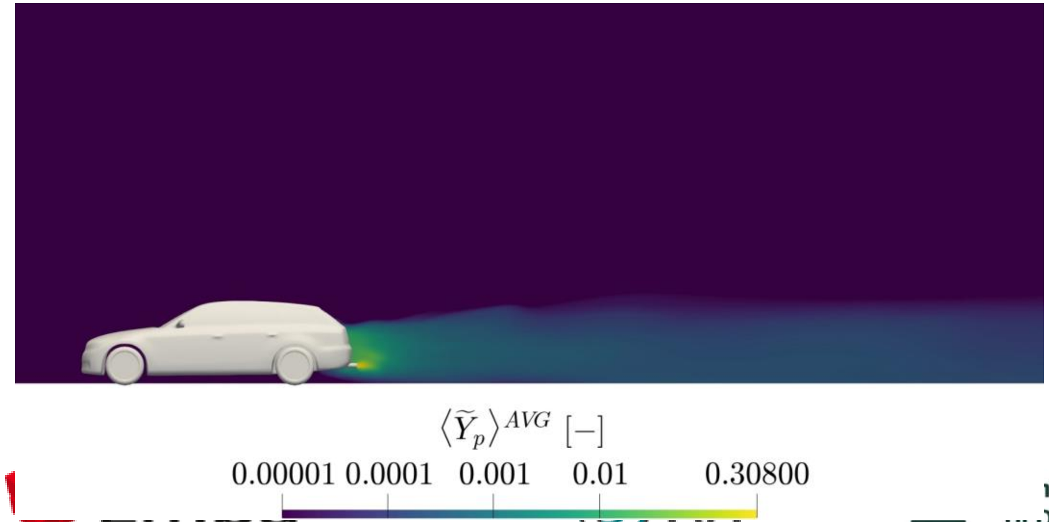
VTT

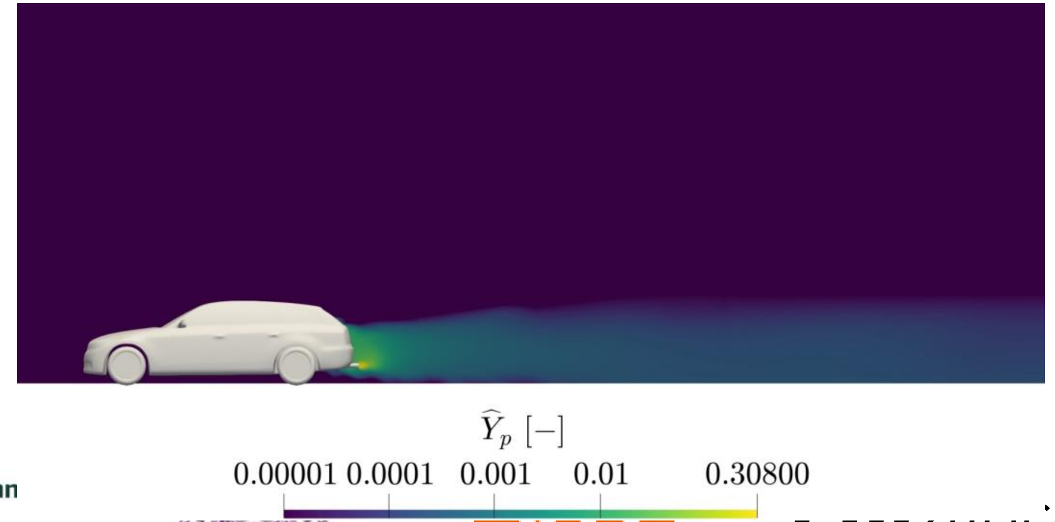
ETH zürich

Consistency of pollutant concentration fields

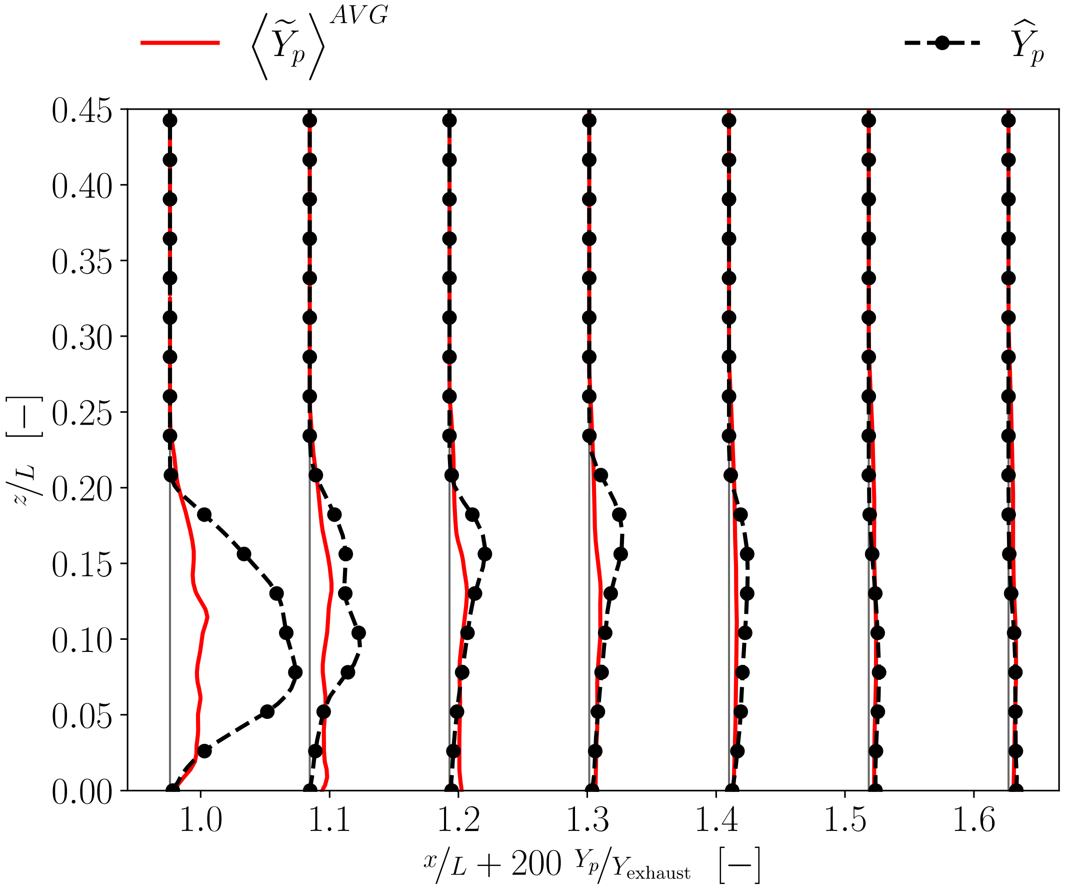


- Analogous to velocity
- Consistency is achieved between averaged LES and URANS pollutant concentrations

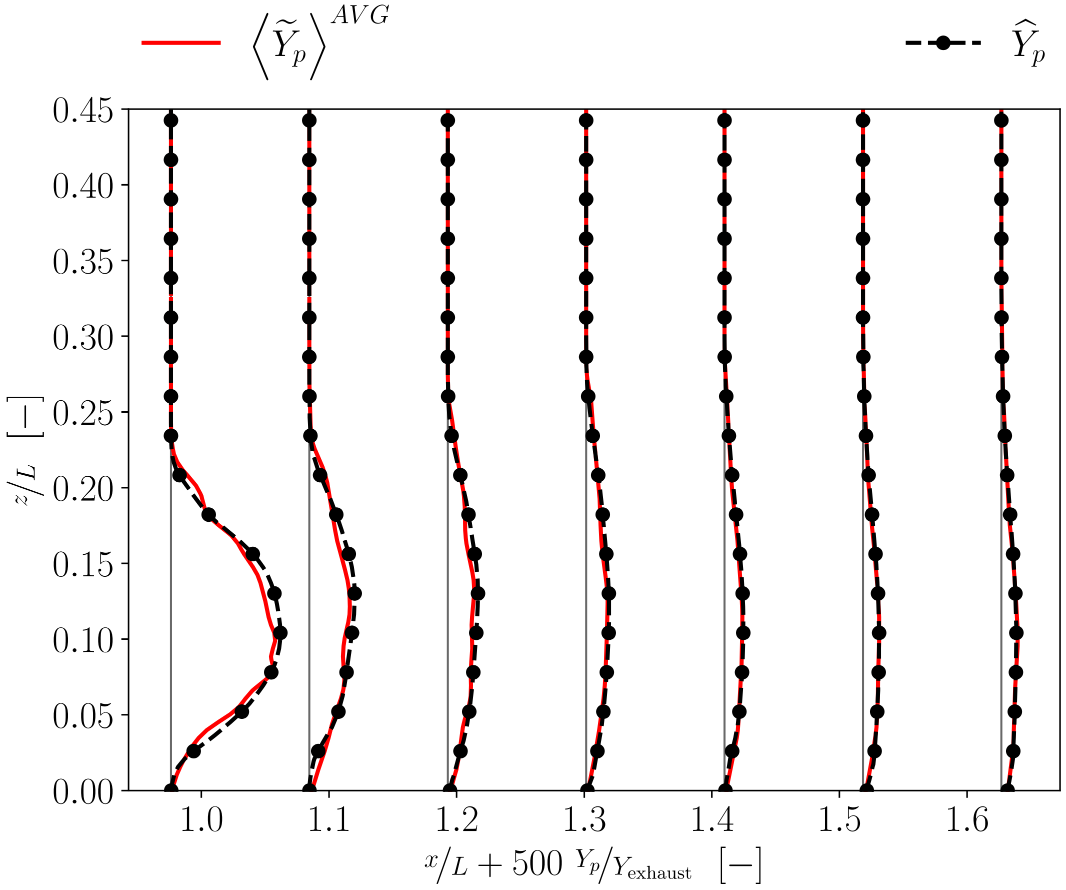




Consistency of pollutant concentration fields



Before coupling (standalone simulations)



After coupling (hybrid simulation)

Empa Materials Science and Technology
ivl Swedish Environmental Research Institute
Ministry of Environment of Denmark Environmental Protection Agency
VTT
ETH zürich

Dissertation Justin Plogmann

URANS simulations of vehicle exhaust plumes with insight on remote emission sensing

↓

Development of a consistent dual-mesh framework for hybrid LES/RANS simulations

↓

Hybrid LES/RANS simulations of vehicle exhaust plumes
Implications for remote emission sensing

↓

Sparse data assimilation for the optimization of unsteady flow problems

Focus: Simulations and specific evaluations of measurement data

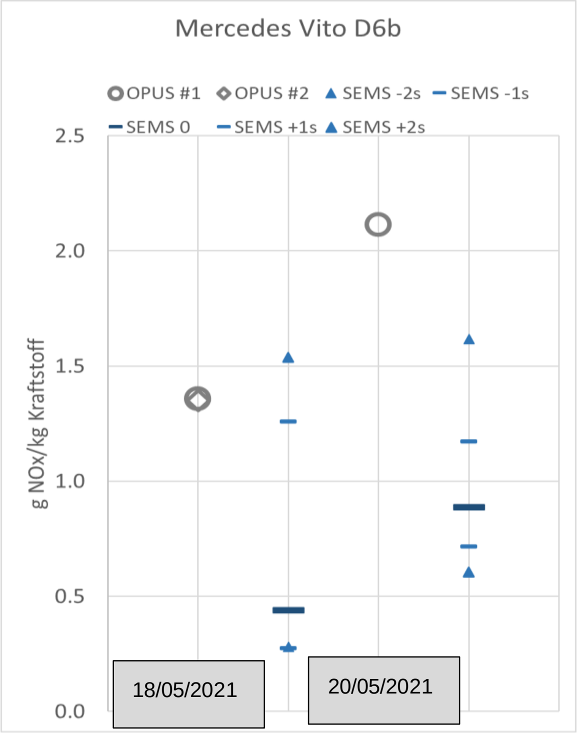
- WP 1: Numerical Simulation of the dispersion of a pollutant in the vehicle
- WP2: Relation of RES measured data to the actual vehicle emission
- WP 3: Potential of RES measurements for determining aging of vehicles' exhaust aftertreatment systems in the field
- WP 4: Technical exchange with the other countries in the project, other projects. Integration of the Swiss measurements in the CONOx database

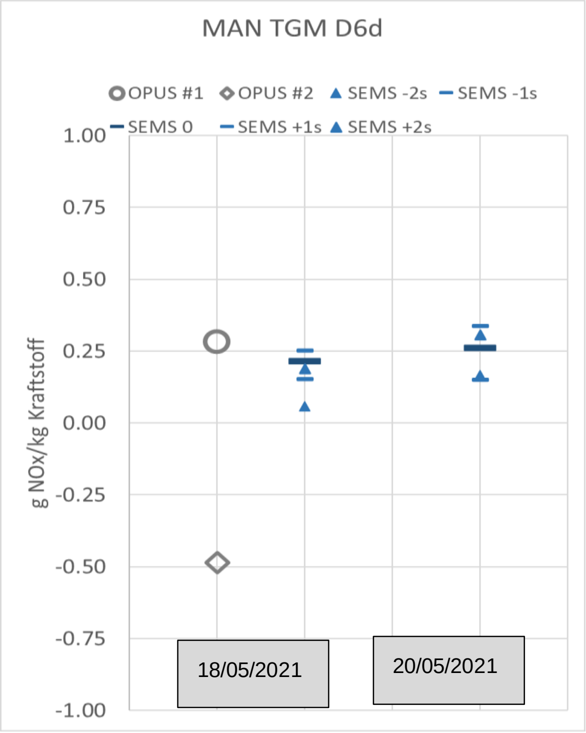
Empa Materials Science and Technology
ivl Swedish Environmental Research Institute
Ministry of Environment of Denmark Environmental Protection Agency
VTT
ETH zürich

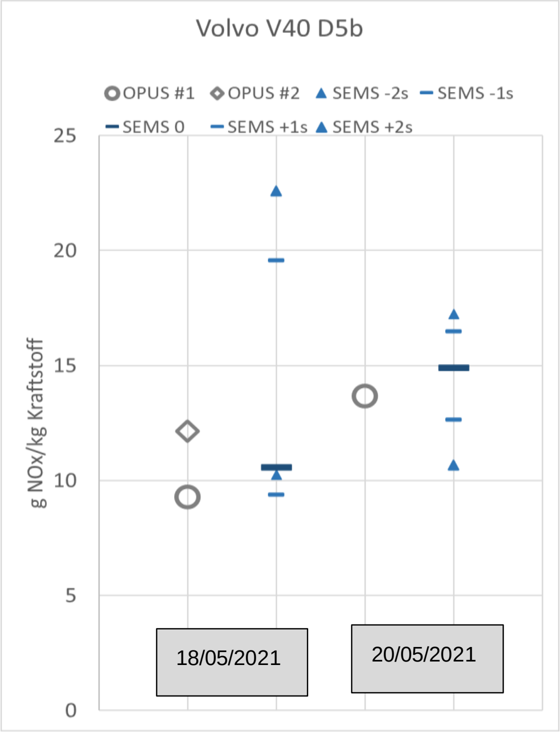
ADVANCED MOTOR FUELS IEA-AMF

Comparison of RES to vehicle on board/portable emission measurements (SEMS)

Task 61







Empa Materials Science and Technology

ivl Swedish Environmental Research Institute

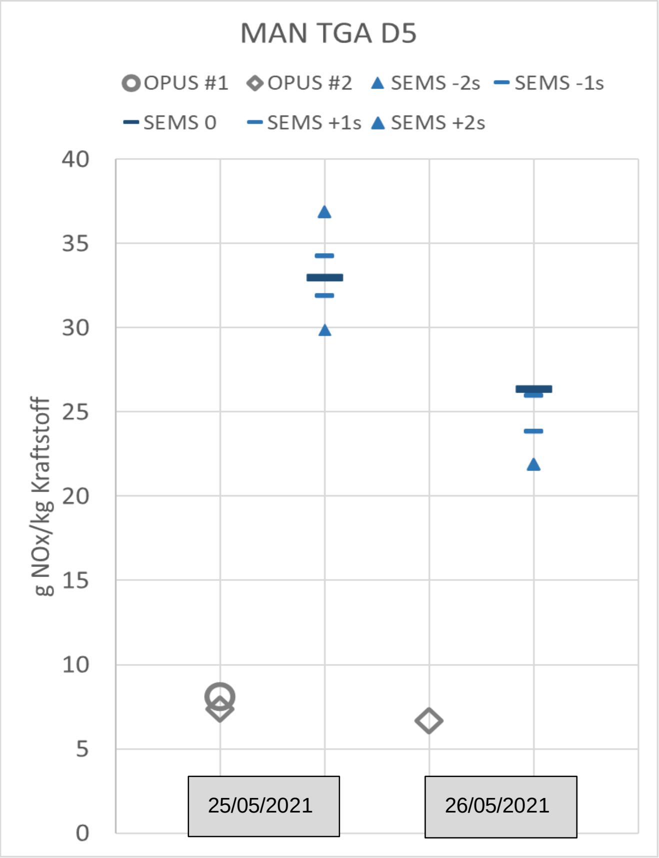
Ministry of Environment of Denmark Environmental Protection Agency

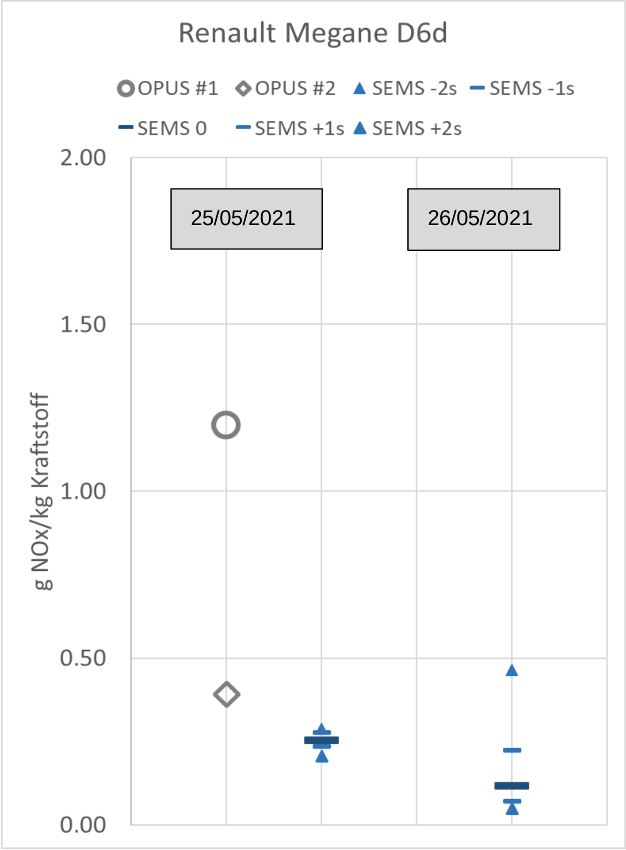
VTT

ETH zürich

High discrepancies for low emitting vehicles (according to Euro 6)

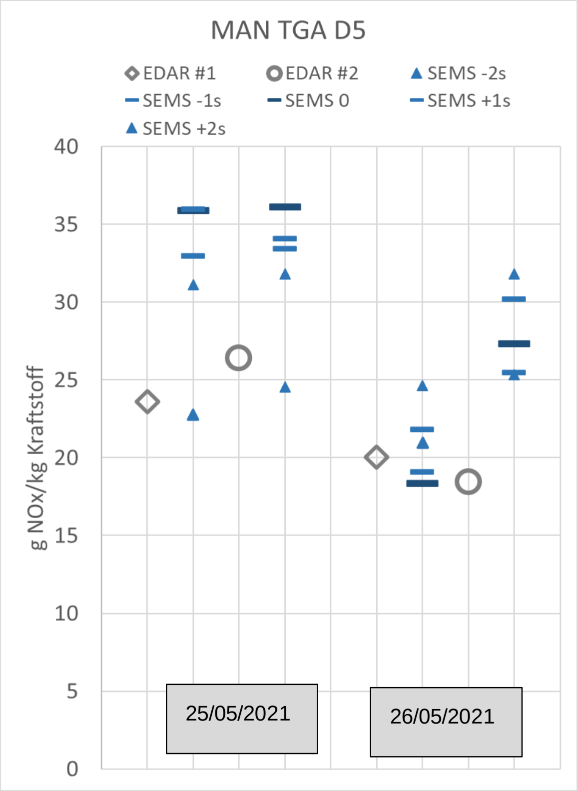
Task 61

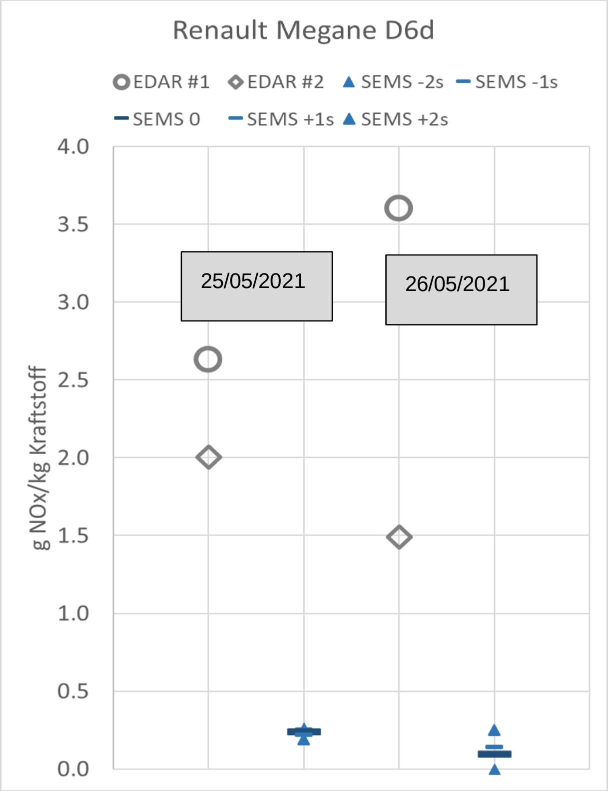




Empa Materials Science and Technology · ivl Swedish Environmental Research Institute · Ministry of Environment of Denmark Environmental Protection Agency · VTT · ETH zürich

Diagram on the left: very good correlation of RES and SEMS,





Task 61

Empa
Materials Science and Technology

ivl
Swedish Environmental Research Institute

Ministry of Environment of Denmark
Environmental Protection Agency

VTT

ETH zürich

Focus: Simulations and specific evaluations of measurement data

- WP 1: Numerical Simulation of the dispersion of a pollutant in the vehicle
- WP2: Relation of RES measured data to the actual vehicle emission
- WP 3: Potential of RES measurements for determining aging of vehicles' exhaust aftertreatment systems in the field
- WP 4: Technical exchange with the other countries in the project, other projects. Integration of the Swiss measurements in the CONOx database

Empa Materials Science and Technology

ivl Swedish Environmental Research Institute

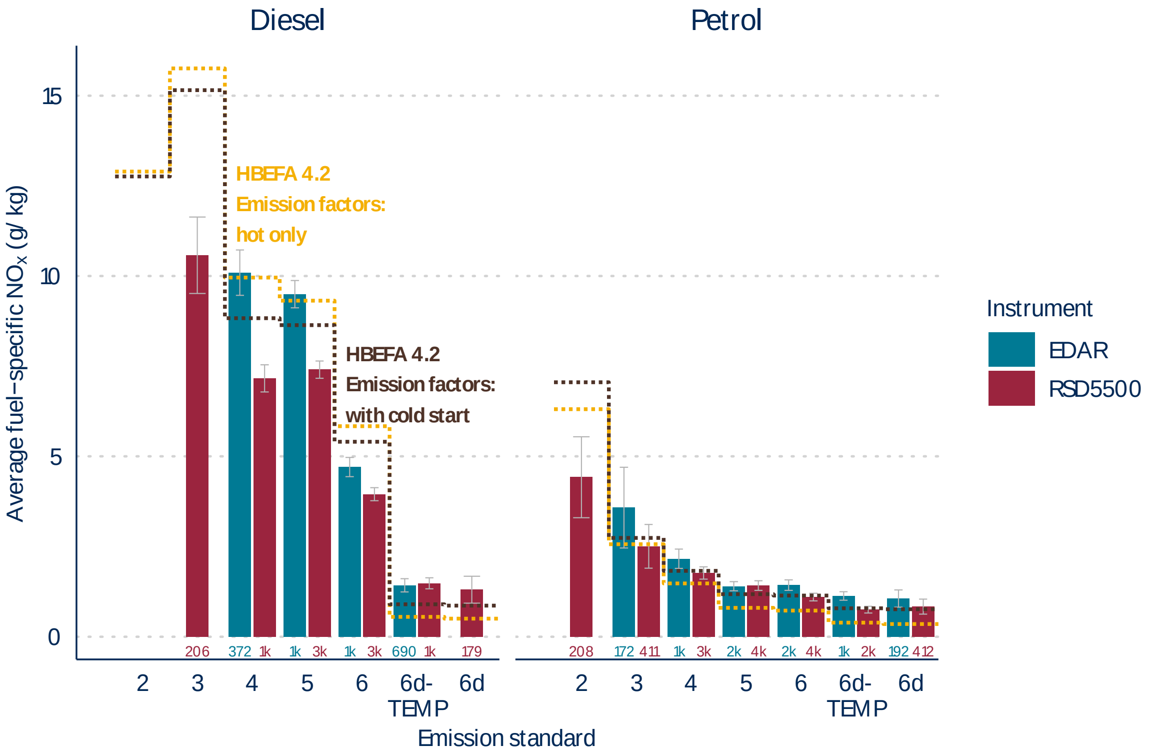
Ministry of Environment of Denmark
Environmental Protection Agency

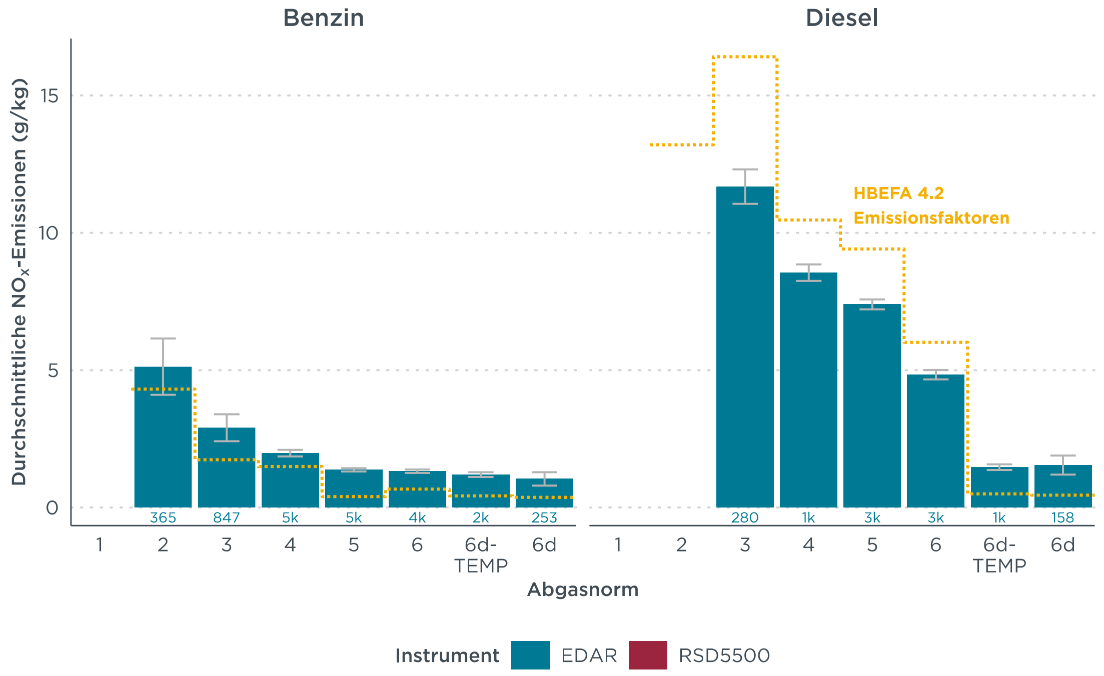
VTT

ETH zürich

Measured values by RES near to the HBEFA 4.2 emission factors

Task 61





Empa Materials Science and Technology

ivl Swedish Environmental Research Institute

Ministry of Environment of Denmark Environmental Protection Agency

VTT

ETH zürich

Simulations show clearly, that the emission information is in the first 1-3m in the vehicle wake (of light duty vehicle)

- Pollutant concentrations in the core exhaust plume are only weakly affected by vehicle movement and/or environmental parameters.
- Careful application of the RES has the potential of characterizing accurately the vehicle emissions.
- While this is clear for light duty vehicles, serious doubts can be addressed towards heavy duty vehicles given the relative large distance between the exhaust pipe exit and the vehicle end.
- Die accuracy of chasing measurements is also under scrutiny.
- Calibration and use of RES is rather for a specialized group of technicians.
- Quantification of the emission of very low emitting vehicles by RES is inaccurate.
- Measurement of NO_2 is imprecise.