Electronic Supplementary Information (ESI):

Particle Emissions of a Heavy-Duty Engine Fueled with Polyoxymethylene Dimethyl Ethers (OME)

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Measurement methods of OME values

| Parameter                                | Value      | Method                          |
|------------------------------------------|------------|---------------------------------|
| Cetane number                            | 68.8       | DIN EN 17155 :2018              |
| Oxygen content in % (w/w)                | 45.0       | DIN 51732 :2014 mod.            |
| Sulfur content in mg/kg                  | < 5        | DIN EN ISO 20884 :2011          |
| Lower heating value in MJ/kg             | 19.21      | DIN 51900-2 :2003 mod.          |
| Density (15°C at 1 bar) in kg/dm\textsuperscript{3} | 1057.1     | DIN EN ISO 12185 :1997         |
| Boiling range at 1 bar in °C             | 144.9 – 242.4 | DIN EN ISO 3405 :2011         |
| Flash point at 1 bar in °C               | 65.0       | DIN EN ISO 2719 :2016           |
| Cold Filter Plugging Point in °C         | -40        | DIN EN 116 :2018                |
| Cloud Point in °C                        | -38        | DIN EN 23015 :1994              |
| Kinematic viscosity at 40°C in mm\textsuperscript{2}/s | 1.082     | DIN EN ISO 3104 :1999          |
| Lubricity – HFFR at 60°C in µm            | 320        | DIN EN ISO 12156-1 :2016        |
| Formaldehyde content in mg/kg            | 233        | ASG 1855 Voltammetry            |

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Properties of the test engine

| Parameter                              | Value                                      |
|----------------------------------------|--------------------------------------------|
| Number of cylinders                    | 6 (inline)                                 |
| Displacement                           | 12,419 cm\textsuperscript{3}               |
| Bore                                   | 126 mm                                     |
| Stroke                                 | 166 mm                                     |
| Power                                  | 294 kW                                     |
| Compression ratio                      | 18 : 1                                     |
| Number of valves per cylinder          | 4 (2 inlet / 2 exhaust)                    |
| Charge                                 | Two-stage waste-gate turbocharger          |
| Exhaust gas recirculation              | High-pressure & cooled                     |
| Injection system                       | Common Rail (max. 1800 bar)                |
| Hydraulic nozzle flow rate             | Diesel: 1,300 cm\textsuperscript{3} / 30 s (at 100 bar) |
|                                        | OME: 1,835 cm\textsuperscript{3} / 30 s (at 100 bar) |
Properties of the aftertreatment system components

Table 3. Properties of the ATS components provided by VT Vitesco Technologies Emitec GmbH in downstream order. The value of the platinum group metals (PGM) density represents the total quantity of the precious metal content of platinum (Pt) and palladium (Pd). (*) The value of the open frontal area (OFA) bases on the following assumptions: coating of the DOC is 150 g/dm³, coating of the Hyd is 60 g/dm³ and coating of the SCR is 200 g/dm³, with a wash-coat density of 1.35 g/cm³. (***) In some test runs with OME, the DPF is removed. The DPF had a mileage of about 500 km in diesel operation before the test runs.

| Component | Catalytic coating | PGM in g/ft³ | Cell density in cpsi | Diameter in mm | Length in mm | Volume in dm³ | Carrier material | Carrier structure | OFA (*) |
|-----------|------------------|--------------|---------------------|----------------|--------------|--------------|-----------------|------------------|---------|
| Hyd       | TiO₂             | -            | N/A                 | 174.6          | 60           | 1.43         | Metal           | 300/600 LSPE     | 89%     |
| SCR       | CuZe             | -            | N/A                 | 300            | 3 x 101.5    | 21.5         | Metal           | 600 CS           | 79%     |
| ASC       | Pt               | 3            | 60                  | 300            | 300          | 90           | 6.4             | Metal            | 78%     |
| DOC       | Pt, Pd (1 : 1)   | 35           | 300                 | 300            | 100          | 10.6         | Metal           | 300/600 LS       | 82%     |
| DPF (**)  | Uncoated         | None         | 300                 | 305            | 381          | 27.8         | Cordierite      | Symmetrical      | 83%     |
| Hyd       | TiO₂             | -            | N/A                 | 174.6          | 60           | 1.43         | Metal           | 300 PE           | 89%     |
| SCR       | CuZe             | -            | 400                 | 300            | 4 x 101.5    | 28.8         | Metal           | E400             | 77%     |

Scheme of the test bench setup

Figure 1. Test bench setup. The raw exhaust sampling point was located approx. 0.5 m downstream of the second turbocharger; the tailpipe sampling point was located approximately 50 mm downstream of the ATS.
### Chronological order of test runs

Table 4. Chronological order of the test runs and the respective setup. (*) marks the last test run of the day, with the next test run happening on another day. (**) The test runs of WHSC and WHTC with DPF happened between the cleaning process after the fuel change and the removal of the DPF.

| Chronological order | Removal of volatile fraction | Dilution | Sampling point | Urea dosing |
|---------------------|------------------------------|----------|----------------|-------------|
|                     | With CS | w/o CS | One-stage | Two-stage | Raw exhaust | Tailpipe | With dosing | w/o dosing |
| 1                   | X       | X      | X         | X         |             |         |             |           |
| 2                   | X       | X      | X         | X         |             |         |             |           |
| 3                   | X       | X      | X         | X         |             |         |             |           |
| 4                   | X       | X      | X         | X         |             |         |             |           |
| 5                   | X       | X      | X         | X         |             |         |             |           |
| 6 (*)               | X       | X      | X         | X         |             |         |             |           |
| 7                   | X       | X      | X         | X         |             |         |             |           |
| 8                   | X       | X      | X         | X         |             |         |             |           |
| 9                   | X       | X      | X         | X         |             |         |             |           |

**Comparison between diesel and OME: raw exhaust**

**Change from diesel to OME: change of the injectors; removal of the DPF (**)**

**Cleaning of the impactor**

**Investigation on OME: one-stage dilution**

**Investigation on urea dosing**

### Step sizes of the DMA

| Step size (nm) | 6.38 nm | 6.61 nm | 6.85 nm | 7.10 nm | 7.37 nm | 7.64 nm | 7.91 nm | 8.20 nm | 8.51 nm | 8.82 nm | 9.14 nm | 9.47 nm | 9.82 nm | 10.2 nm | 10.6 nm | 10.9 nm | 11.3 nm | 11.8 nm | 12.2 nm | 12.6 nm | 13.1 nm | 13.6 nm | 14.1 nm | 14.6 nm | 15.1 nm | 15.7 nm | 16.3 nm | 16.8 nm | 17.5 nm | 18.1 nm | 18.8 nm | 19.5 nm | 20.2 nm | 20.9 nm |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
Calculation of particle losses†

Maximum tube Reynolds number and maximum particle Reynolds number (according to Hinds (1))

The following calculations describe the respective maximum or minimum of each value and therefore enable the decision of whether the flow is laminar or turbulent.

Temperature $T$: 293.15 K
Pressure $p$: 101.3 kPa
Tube diameter $d_t$: 0.006 m
Air velocity $v_a$: 5.895 m/s
Particle diameter $d_p$: 0.23 µm
Particle velocity $v_p$: 5.895 m/s

Air density $\rho_a$:
$$\rho_a = 1.293 \cdot \frac{273.15}{T} \cdot \frac{p}{1013} = 1.2048 \text{ kg/m}^3$$

Air dynamic viscosity $\mu_a$:
$$\mu_a = 0.0000178 \cdot \left(\frac{T}{273.15}\right)^{1.5} \cdot \frac{393.396}{T + 120.246} = 1.8071 \cdot 10^{-5} \text{ Pa} \cdot \text{s}$$

Particle Reynolds number $Re_p$:
$$Re_p = 0.000001 \cdot \rho_a \cdot d_p \cdot \frac{v_p}{\mu_a} = 0.0904$$

According to Hinds, the flow is laminar for $Re_p < 0.1$.

Tube Reynolds number $Re_t$:
$$Re_t = \rho_a \cdot d_t \cdot \frac{v_a}{\mu_a} = 2358$$

According to Hinds, the flow is laminar for $Re_t < 2000$, but not turbulent as long as $Re_t < 4000$ (1).

Since $Re_p$ decreases for smaller particles and higher aerosol temperature, and $Re_t$ decreases with higher aerosol temperature, the assumption of laminar flow in all parts of the sampling system is valid.

Gravitational settling in the inlet (according to Willeke & Baron(2))

The following calculations describe the respective maximum or minimum of each value and therefore lead to the minimum penetration rate through the inlet.

Air dynamic viscosity $\mu_a$: 1.8071 \cdot 10^{-5} \text{ Pa} \cdot \text{s}
Tube diameter $d_t$: 0.006 m
Air velocity $v_a$: 5.895 m/s
Particle diameter $d_p$: 0.23 µm
Particle density $\rho_p$: 1000 kg/m³
Inlet length $l_i$: 0.3 m
Sampling angle $\theta$: 45°
Velocity ratio $R$: 1 (isokinetic)
Flow Reynolds number $Re_t$: 2358

Slip correction factor $S$:
$$S = 1 + \frac{2}{p \cdot d_p \cdot 0.752} \cdot 6.32 + 2.01$$

Setting velocity $v_s$:
$$v_s = \rho_p \cdot d_p^2 \cdot 0.000000000001 \cdot 9.81 \cdot \frac{S}{18 \cdot \mu_a} = 2.8 \cdot 10^{-6} \text{ m/s}$$

Stokes number $St$:
$$St = \rho_p \cdot d_p^2 \cdot 0.000000000001 \cdot \frac{S}{18 \cdot \mu_a} \cdot \frac{R}{d_t} = 0.0003$$

Gravitational deposition parameter $g_d$:
$$g_d = l_i \cdot \frac{v_s}{v_a} \cdot d_t$$

K($\theta$):
$$K(\theta) = \sqrt{g_d \cdot St \cdot Re_t^{-0.25} \cdot \cos\left(\frac{\theta}{180}\right)}$$

Penetration rate $r_p$:
$$r_p = e^{-\left(4.7 \cdot K(\theta)^{0.75}\right)} = 0.9992$$

Since $r_p$ increases for smaller particles and higher aerosol temperature, the neglect of gravitational settling in the inlet is valid.

†The calculations were performed using Matlab R2019b. Therefore it used more digits than indicated in this document. The EXCEL-Tool "aerocalc" by Paul Baron was used for the specific formulas.
**Sedimentation (according to Willeke & Baron (2))**

The following calculations describe the respective maximum or minimum of each value and therefore lead to the minimum penetration rate inside the tubing.

| Parameter                  | Value                      |
|----------------------------|----------------------------|
| Particle diameter dₚ       | 0.23 µm                    |
| Particle density ρₚ        | 1000 kg/m³                 |
| Tube diameter d₁           | 0.006 m                    |
| Tube length l₁             | 4.37 m                     |
| Incline angle δ            | 0°                         |
| Mean flow velocity vₛ      | 5.895 m/s                  |
| Flow Reynolds number Reₖ  | 2358                       |
| Slip correction factor S   | 1.7551 (for dₚ = 0.23 µm)  |
| Setting velocity vₛ        | 2.8·10⁻⁶ m/s               |

Intermediate number k₁:

\[ k_1 = \cos \left( \pi \cdot \frac{\delta}{180} \right) \cdot 3 \cdot v_s \cdot \frac{l_1}{4 \cdot d_1 \cdot v_a} \]

Intermediate number k₂:

\[ k_2 = \arcsin \left( \frac{1}{k_1^3} \right) \]

Penetration rate \( r_p \):

\[ r_p = 1 - 2\pi \cdot \sqrt{1 - \left( \frac{1}{k_1^3} \right)} + k_2 - \left( \frac{1}{k_1^3} \right) \cdot \sqrt{1 - k_2^3} = 0.9996 \]

Since \( r_p \) increases for smaller particles and higher aerosol temperature, the neglect of gravitational settling in the tubing is valid.

**Bent tubing (according to Willeke & Baron (2))**

The following calculations describe the respective maximum or minimum of each value and therefore lead to the minimum penetration rate through bent tubing.

| Parameter                  | Value                      |
|----------------------------|----------------------------|
| Particle diameter dₚ       | 0.23 µm                    |
| Stokes number St           | 0.0003                     |
| Flow Reynolds number Reₖ  | 2358                       |
| Angle of bend ψ            | 90°                        |

Penetration rate \( r_p \):

\[ r_p = 1 - St \cdot \gamma \cdot \frac{\pi}{180} = 0.9993 \]

Since \( r_p \) increases for smaller particles and higher aerosol temperature, the neglect of losses in bent tubing is valid.

**Coagulation (according to Willeke & Baron (2))**

The following calculations describe the respective maximum or minimum of each value and therefore lead to the maximum coagulation rate. Furthermore, the initial particle concentration considers monodisperse aerosol of the total concentration.

Upper particle diameter \( d_{pu} \): 0.23 µm
Lower particle diameter \( d_{pu} \): 0.006 µm
Initial particle concentration \( PN \): 10³¹ 1/m³
Coagulation coefficient \( c \): 5.6·10⁻¹⁶ m³/s
Time \( t \): ~1 s
(tubing length: 4.3 m, velocity: 5.9 m/s)

Final particle concentration \( PN_f \):

\[ PN_f = \frac{PN}{1 + PN \cdot c \cdot t} = 9.9443 \cdot 10^{-12} \text{ m}^3 \]

Final particle size \( d_{fu} \) for \( d_{pu} \):

\[ d_{fu} = d_{pu} \left( \frac{PN}{PN_{fu}} \right) ^{\frac{1}{3}} = 0.2304 \, \mu\text{m} \]

Final particle size \( d_{fu} \) for \( d_{pu} \):

\[ d_{fu} = d_{pu} \left( \frac{PN}{PN_{fu}} \right) ^{\frac{1}{3}} = 0.0060 \, \mu\text{m} \]

Since the aerosol is polydisperse with lower total particle concentrations and the dwell time is less than one second, the neglect of coagulation is valid.

**Thermophoretic velocity (according to Hinds (1) and Willeke & Baron (2))**

The following calculations describe the respective maximum or minimum of each value and therefore lead to the maximum thermophoretic velocity tubing.

Temperature of particle \( T_p \): 693.15 K
Pressure \( p \): 101.3 kPa
Particle diameter \( d_p \): 0.23 µm
Particle thermal conductivity \( k \): 4.2 W/m·K (carbon)
Thermal gradient \( \Delta T \): 4000 K/m
Air density \( \rho_{a,h} \): 0.5095 kg/m³
Air dynamic viscosity \( \mu_{a,h} \): 3.3393·10⁻⁵ Pa·s
Slip correction factor S: 1.7551 (for \( d_p = 0.23 \mu m \))

Mean free path \( \lambda \):

\[ \lambda = 0.00674 \cdot 0.0001 \cdot \frac{T_p}{296.15} \cdot \frac{1 + \frac{110.4}{p}}{1 + \frac{110.4}{296.15}} \]

Intermediate factor H:

\[ H = \frac{1}{1 + 6 \cdot \frac{\lambda}{d_p} - 0.000001} \cdot \left( \frac{0.026}{\kappa} + 4.4 \cdot \frac{\lambda}{d_p} \cdot 0.000001 \right) \]

\[ H = \frac{1 + 2 \cdot \frac{0.026}{\kappa} + 8.8 \cdot \frac{\lambda}{d_p} \cdot 0.000001}{1 + 6 \cdot \frac{\lambda}{d_p} - 0.000001} \]

Thermophoretic velocity \( v_T \):

\[ v_T = 3 \cdot \mu_{a,h} \cdot S \cdot H \cdot \frac{\Delta T}{2 \cdot \rho_{a,h} \cdot T_p} = 7.4375 \cdot 10^{-5} \frac{m}{s} \]
Since $v_T$ decreases for lower aerosol temperature and lower temperature gradients, the neglect of thermophoretic losses is valid.

**Diffusional losses in a cylindrical tube-fraction passing through tube under laminar flow (according to Willeke & Baron (2))**

Since the tubing length between the catalytic stripper and the SMPS is the dominant part in this calculation, the temperature inside the tubing is assumed to be 20°C. The maximum deviation in penetration efficiency between an aerosol temperature of 20°C and 220°C is less than 1.06% absolute for a particle diameter of 6 nm.

Temperature $T$: 293.15 K
Pressure $p$: 101.3 kPa
Particle diameter $d_p$: from 0.006 µm to 0.23 µm
Tube diameter $d_t$: 0.006 m
Tube length $l_t$: 4.37 m
Air flow rate $V_a$: 1.667 $\cdot$ 10^{-4} m³/s
Air density $\rho_a$: 1.2048 kg/m³
Air dynamic viscosity $\mu_a$: 1.8071 $\cdot$ 10^{-5} Pa·s
Slip correction factor $S$: depending on $d_p$

Diffusion coefficient $\beta$:

$$\beta = 1.38 \cdot 10^{-23} \cdot \frac{T}{3 \cdot \pi \cdot \mu_a \cdot d_p} \cdot 0.000001$$

$Hinds$:

$$\mu_{Hinds} = \beta \cdot \frac{l_t}{V_a}$$

Penetration rate $r_p$:

$$r_p = 1 - 5.5 \cdot (\mu_{Hinds})^2 + 3.77 \cdot \mu_{Hinds}$$

**Particle losses in the ejector diluters (according to Giechaskiel et al. (3))**

The transportation losses of the ejector diluters were assumed to be 5% for each diluter and for any particle diameter, according to the measurements of Giechaskiel et al. (3).

**Electrostatic losses**

Transport losses due to electrostatic fields were neglected due to the usage of stainless steel wherever possible and an intermediate connection using Tygon tubing. This polymer is known as a tubing material having lower electrostatic losses than other kinds of tubing (4–6).

**Particle losses inside the catalytic stripper**

The manufacturer of the catalytic stripper (Catalytic Instruments GmbH & Co. KG) provide in the manual, penetration efficiency data at nominal flow (10 l/min):

| $D_p$ (nm) | $F$ | $D_p$ (nm) | $F$ | $D_p$ (nm) | $F$ |
|-----------|-----|-----------|-----|-----------|-----|
| 3.55      | 0.0017 | 7.30     | 0.03 | 12.10    | 0.15 |
| 3.56      | 0.0017 | 7.31     | 0.03 | 12.11    | 0.15 |
| 3.57      | 0.0017 | 7.32     | 0.03 | 12.12    | 0.15 |
| 3.58      | 0.0017 | 7.33     | 0.03 | 12.13    | 0.15 |

Figure 2 shows the calculated penetration efficiencies of the purpose-built sampling systems with and without the CS or the second dilution stage. The results of the PSD in this work use the PCRF of these calculations. Furthermore, the “Aerosol Instrument Manager” software by TSI includes the option of considering the diffusion losses inside the SMPS and a multiple charge correction. The evaluations in this study include these considerations.

**Calculated particle losses**

- one-stage w/o CS
- two-stage w/o CS
- one-stage with CS
- two-stage with CS

**Considered losses:**
- Brownian diffusion
- Ejector diluters
- Catalytic stripper

Figure 2. Calculated particle losses. The losses due to Brownian diffusion are based on calculations according to Hinds (1) with the assumption of a laminar flow inside the tubing. The losses of each ejector diluter were assumed to be 5% according to Giechaskiel et al. (3). The manufacturer of the catalytic stripper determined the respective penetration efficiency at a nominal flow rate of 10 l/min.
References

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