Electronic Supplementary Information (ESI): Particle Emissions of a Heavy-Duty Engine Fueled with Polyoxymethylene Dimethyl Ethers (OME)

Alexander Daniel Gelner[a], Dieter Rothe[b], Carsten Kykal[c], Martin Irwin[d], Alessandro Sommer[a], Christian Pastötter[b] and Georg Wachtmeister[a]

[a] Technical University of Munich, Institute of Internal Combustion Engines, Schragenhofstraße 31, 80992 Munich, Germany.
[b] MAN Truck & Bus SE, Vogelweiherstraße 33, Nuremberg, Germany.
[c] TSI GmbH,Neuköllner Straße 4, 52068 Aachen, Germany.
[d] Catalytic Instruments GmbH & Co. KG, Zellerhornstraße 7, 83026 Rosenheim.

Measurement methods of OME values

Table 1. Determined values of OME and the respective measurement method

	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/dm³	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 mm²/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

Properties of the test engine

Table 2. Properties of the test engine MAN D2676LF51. The injectors in OME operation have a higher nozzle flow rate to reduce the combustion duration at high-load points.

Number of cylinders	6 (inline)
Displacement	12,419 cm³
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 cm³ / 30 s (at 100 bar) OME: 1,835 cm³ / 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	TiO_2	-	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	300	300	90	6.4	Metal	E300	78%
DOC	Pt, Pd (1 : 1)	35	300	300	150	10.6	Metal	300/600 LS	82%
DPF (**)	Uncoated	None	300	305	381	27.8	Cordierite	Symmetrical	83%
Hyd	TiO_2	-	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

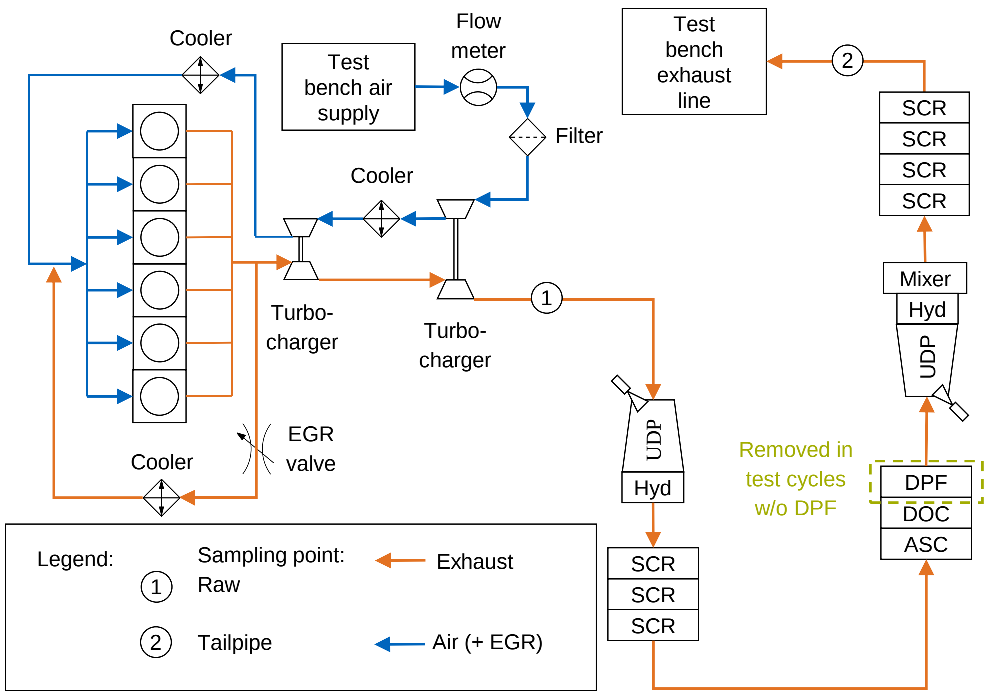

Figure 1. Test bench setup. The raw exhaust sampling point was located approx. 0.5 m downstream of the second turbocharger; the tailpipe sampling point was located approximately 50 mm downstream of the ATS.

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
Comparison between diesel and OME: raw exhaust								
1	X			X	X			X
2		X		X	X			X
Change from diesel to OME; change of the injectors; removal of the DPF (**); cleaning of the impactor								
3	X			X	X			X
4		X		X	X			X
Investigation on OME: one-stage dilution								
5	X		X		X			X
6 (*)		X	X		X			X
7	X		X			X		X
8		X	X			X		X
Investigation on urea dosing								
9	X		X			X	X	

Step sizes of the DMA

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
21.7 nm
22.5 nm
23.3 nm
24.1 nm
25.0 nm
25.9 nm
26.9 nm
27.9 nm
28.9 nm
30.0 nm
31.1 nm
32.2 nm
33.4 nm
34.6 nm
35.9 nm
37.2 nm
38.5 nm
40.0 nm
41.4 nm
42.9 nm
44.5 nm
46.1 nm
47.8 nm
49.6 nm
51.4 nm
53.3 nm
55.2 nm
57.3 nm
59.4 nm
61.5 nm
63.8 nm
66.1 nm
68.5 nm
71.0 nm
73.7 nm
76.4 nm
79.1 nm
82.0 nm
85.1 nm
88.2 nm
91.4 nm
94.7 nm
98.2 nm
101.8 nm
105.5 nm
109.4 nm
113.4 nm
117.6 nm
121.9 nm
126.3 nm
131.0 nm
135.8 nm
140.7 nm
145.9 nm
151.2 nm
156.8 nm
162.5 nm
168.5 nm
174.7 nm
181.1 nm
187.7 nm
194.6 nm
201.7 nm
209.1 nm
216.7 nm
224.7 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 ρ_a:

$$\rho_a = 1.293 \cdot \frac{273.15}{T} \cdot \frac{p}{101.3} = 1.2048 \frac{kg}{m^3}$$

Air dynamic viscosity μ_a:

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

Particle Reynolds number Re_p:

$$Re_p = 0.000001 \cdot \mathrm{\rho_a} \cdot d_p \cdot \frac{v_p}{\mu_a} = 0.0904$$

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

Tube Reynolds number Re_t:

$$Re_t = \mathrm{\rho_a} \cdot d_t \cdot \frac{v_a}{\mu_a} = 2358$$

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 μ_a:	$1.8071 \cdot 10^{-5}$ Pa·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 ρ_p:	1000 kg/m³
Inlet length l_i:	0.3 m
Sampling angle θ:	45°
Velocity ratio R:	1 (isokinetic)
Flow Reynolds number Re_f:	2358

Slip correction factor S:

$$S = 1 + \left(\frac{2}{p \cdot d_p \cdot 0.752}\right) \cdot 6.32 + 2.01 \cdot e^{(-0.1095 \cdot p \cdot 0.752 \cdot d_p)} = 1.7551$$

Setting velocity v_s:

$$\mathrm{v_s} = \mathrm{\rho_p} \cdot \mathrm{d_p^2} \cdot 0.000000000001 \cdot 9.81 \cdot \frac{S}{18 \cdot \mu_a} = 2.8 \cdot 10^{-6} \frac{m}{s}$$

Stokes number St:

$$\mathrm{St} = \mathrm{\rho_p} \cdot \mathrm{d_p^2} \cdot 0.000000000001 \cdot \frac{S}{18 \cdot \mu_a} \cdot v_a \cdot \frac{R}{d_t} = 0.0003$$

Gravitational deposition parameter g_d:

$$\mathrm{g_d} = l_i \cdot \frac{\mathrm{v_s}}{v_a \cdot d_t}$$

K(θ):

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

Penetration rate r_p:

$$\mathrm{r_p} = \mathrm{e}^{-(4.7 \cdot \mathrm{K(\theta)}^{0.75})} = 0.9992$$

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.

Particle diameter d_p:	0.23 µm
Particle density ρ_p:	1000 kg/m³
Tube diameter d_t:	0.006 m
Tube length l_t:	4.37 m
Incline angle δ:	0°
Mean flow velocity v_a:	5.895 m/s
Flow Reynolds number Re_f:	2358
Slip correction factor S:	1.7551 (for d_p = 0.23 µm)
Setting velocity v_s:	$2.8 \cdot 10^{-6}$ m/s

Intermediate number k_1:

$$k_1 = \cos\left(\pi \cdot \frac{\delta}{180}\right) \cdot 3 \cdot v_s \cdot \frac{l_t}{4 \cdot d_t \cdot v_a}$$

Intermediate number k_2:

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

Penetration rate r_p:

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

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.

Particle diameter d_p:	0.23 µm
Stokes number St:	0.0003
Flow Reynolds number Re_f:	2358
Angle of bend γ:	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_{pl}:	0.006 µm
Initial number concentration PN:	10^{13} 1/m³
Coagulation coefficient c:	$5.6 \cdot 10^{-16}$ m³/s
Time t:	~1 s

(tubing length: 4.3 m, velocity: 5.9 m/s)

Final particle concentration PN_f :

$$PN_f = \frac{PN}{1 + PN \cdot c \cdot t} = 9.9443 \cdot 10^{12}\ 1/m^3$$

Final particle size d_{fu} for d_{pu}:

$$d_{fu} = \mathrm{d_{pu}} \cdot \left(\frac{PN}{PN_{fu}}\right)^{\frac{1}{3}} = 0.2304\ \mu m$$

Final particle size d_{fl} for d_{pl}:

$$d_{fl} = \mathrm{d_{pl}} \cdot \left(\frac{PN}{PN_{fu}}\right)^{\frac{1}{3}} = 0.0060\ \mu m$$

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 κ:	4.2 W/m·K (carbon)
Thermal gradient ΔT:	4000 K/m
Air density $\rho_{a,h}$:	0.5095 kg/m³
Air dynamic viscosity $\mu_{a,h}$:	$3.3393 \cdot 10^{-5}$ Pa·s
Slip correction factor S:	1.7551 (for d_p = 0.23 µm)

Mean free path λ:

$$\lambda = 0.000674 \cdot 0.0001 \cdot \frac{T_p}{296.15} \cdot \frac{101.3}{p} \cdot \frac{1 + \frac{110.4}{296.15}}{1 + \frac{110.4}{T_p}}$$

Intermediate factor H:

$$H = \frac{\frac{1}{1 + 6 \cdot \frac{\lambda}{d_p \cdot 0.000001}} \cdot \left(\frac{0.026}{\kappa} + 4.4 \cdot \frac{\lambda}{d_p \cdot 0.000001}\right)}{1 + 2 \cdot \frac{0.026}{\kappa} + 8.8 \cdot \frac{\lambda}{d_p \cdot 0.000001}}$$

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 $\dot{V}_a$:	$1.667 \cdot 10^{-4}$ m³/s
Air density ρ_a:	1.2048 kg/m³
Air dynamic viscosity μ_a:	$1.8071 \cdot 10^{-5}$ Pa·s
Slip correction factor S:	depending on d_p

Diffusion coefficient β:

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

μ_{Hinds}:

$$\mu_{Hinds} = \beta \cdot \frac{l_t}{\dot{V}_a}$$

Penetration rate r_p:

$$r_p = 1 - 5.5 \cdot (\mu_{Hinds})^{\frac{2}{3}} + 3.77 \cdot \mu_{Hinds}$$

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):

Dp, nm	P	Dp, nm	P	Dp, nm	P	Dp, nm	P
3.00	0.01	15.70	0.55	79.10	0.73	399.50	0.75
3.11	0.01	16.30	0.56	82.00	0.73	414.20	0.75
3.22	0.02	16.80	0.57	85.10	0.74	429.40	0.75
3.34	0.02	17.50	0.58	88.20	0.74	445.10	0.75
3.46	0.03	18.10	0.58	91.40	0.74	461.40	0.75
3.59	0.04	18.80	0.59	94.70	0.74	478.30	0.75
3.72	0.05	19.50	0.60	98.20	0.74	495.80	0.75
3.85	0.05	20.20	0.60	101.80	0.74	399.50	0.75
4.00	0.07	20.90	0.61	105.50	0.74	414.20	0.75
4.14	0.08	21.70	0.62	109.40	0.74	429.40	0.75
4.29	0.09	22.50	0.62	113.40	0.74	445.10	0.75
4.45	0.10	23.30	0.63	117.60	0.74	461.40	0.75
4.61	0.11	24.10	0.64	121.90	0.74	478.30	0.75
4.78	0.13	25.00	0.64	126.30	0.74	495.80	0.75
4.96	0.14	25.90	0.65	131.00	0.74	399.50	0.75
5.14	0.16	26.90	0.65	135.80	0.74	414.20	0.75
5.33	0.17	27.90	0.66	140.70	0.74	429.40	0.75
5.52	0.19	28.90	0.66	145.90	0.74	445.10	0.75
5.73	0.21	30.00	0.67	151.20	0.74	461.40	0.75
5.94	0.22	31.10	0.67	156.80	0.74	478.30	0.75
6.15	0.24	32.20	0.68	162.50	0.74		
6.38	0.26	33.40	0.68	168.50	0.74		
6.61	0.27	34.60	0.69	174.70	0.74		
6.86	0.29	35.90	0.69	181.10	0.74		
7.11	0.30	37.20	0.69	187.70	0.74		
7.37	0.32	38.50	0.70	194.60	0.74		
7.64	0.33	40.00	0.70	201.70	0.74		
7.92	0.35	41.40	0.70	209.10	0.75		
8.21	0.36	42.90	0.70	216.70	0.75		
8.51	0.38	44.50	0.71	224.70	0.75		
8.82	0.39	46.10	0.71	232.90	0.75		
9.14	0.40	47.80	0.71	241.40	0.75		
9.48	0.42	49.60	0.71	250.30	0.75		
9.82	0.43	51.40	0.72	259.50	0.75		
10.18	0.44	53.30	0.72	269.00	0.75		
10.56	0.45	55.20	0.72	278.80	0.75		
10.94	0.46	57.30	0.72	289.00	0.75		
11.34	0.47	59.40	0.72	299.60	0.75		
11.76	0.48	61.50	0.73	310.60	0.75		
12.19	0.49	63.80	0.73	322.00	0.75		
13.10	0.51	66.10	0.73	333.80	0.75		
13.60	0.52	68.50	0.73	346.00	0.75		
14.10	0.53	71.00	0.73	358.70	0.75		
14.60	0.54	73.70	0.73	371.80	0.75		
15.10	0.54	76.40	0.73	385.40	0.75		

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.

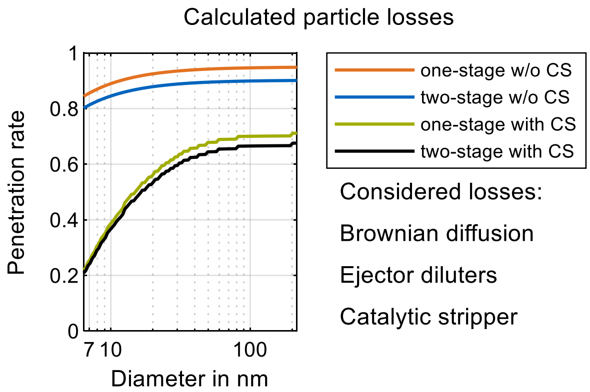

Figure 2. Calculated particle losses. The losses due to Brownian diffusion are based on calculations according to Hinds (1) with the assumption of a laminar flow inside the tubing. The losses of each ejector diluter were assumed to be 5% according to Giechaskiel et al. (3). The manufacturer of the catalytic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

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