Molecular characterization of the gas/particle interface of soot sampled from a diesel engine using a titration method

A. Tapia[1], M. S. Salgado[1*], María Pilar Martín[1], M. Lapuerta[2], J. Rodríguez-Fernández[2], M. J. Rossi[3] and B. Cabañas[1]

[1]*Universidad de Castilla La Mancha. Departamento de Química Física, Facultad de Ciencias y Tecnologías Químicas. Avda Camilo José Cela s/n, 13071 Ciudad Real, Spain*

[2]*Universidad de Castilla la Mancha. Grupo de Combustibles y Motores. Escuela Técnica Superior de Ingenieros Industriales. Avda Camilo José Cela 10,13071 Ciudad Real, Spain.*

[3]*Labor für Atmosphärenchemie (LAC), Paul Scherrer Institute (PSI), OBBA006, CH-5232, Villigen PSI, Switzerland*

[*]Corresponding author. Tel*: (+34) 925295300-3450*

E-mail: sagrario.salgado@uclm.es (Sagrario Salgado)

NUMBER OF PAGES (INCLUDING THIS):10

NUMBER OF FIGURES: 13

NUMBER OF TABLES: 3

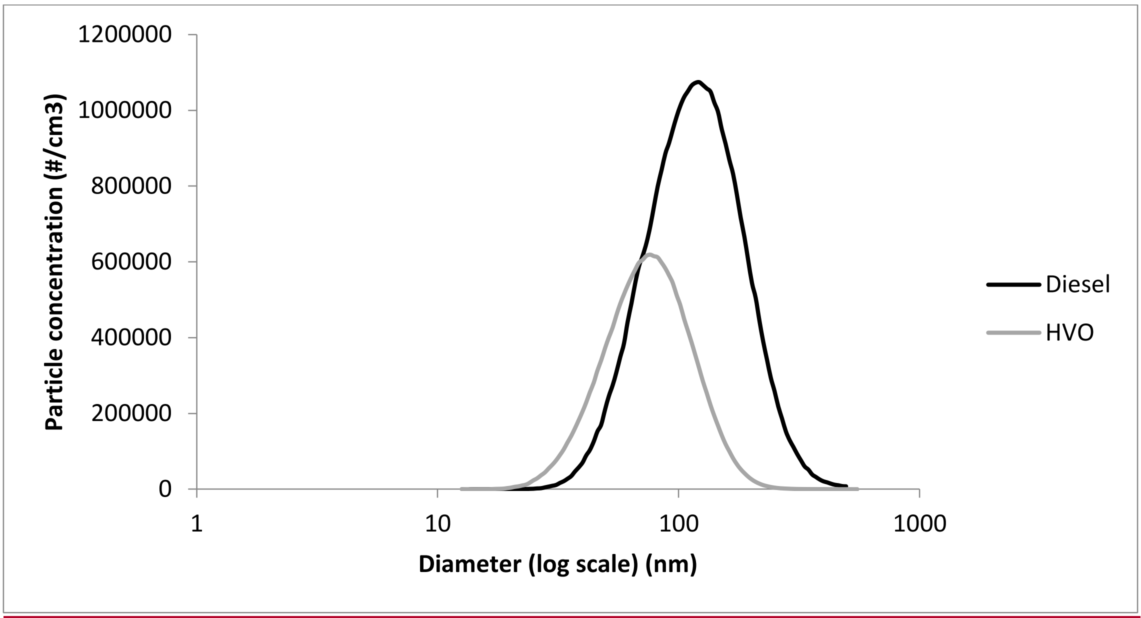

Figure 1S. Particle size distribution of the recovered diesel and HVO soot samples measured using a Scanning Mobility Particle Sizer (SMPS) device with Differential Mobility Analyser (DMA).

Table 1S. Parameters defining running conditions in the engine mode (U9) selected for the experiments.

Measured variables	Units	U9 Mode
Engine speed	rpm	1667
Effective torque	Nm	78
EGR Ratio	%	22-23
Air flow	kg/h	≈78
Start of main injection	ºCA (aTDC)	5
Start of pilot injection	ºCA (bTDC)	12.7
Fuel injected during pilot injection	µL/inj	1.86
Injection pressure	bar	660

Table 2S. Physico-chemical properties of pure fuels.

Properties	Diesel	HVO
Density at 15 ºC / kg m^{-3}	811	779.6
Viscosity at 40 ºC / cSt	2	2.99
Lower heating value/ MJ kg^{-1}	43.13	43.955
Lubricity (WS1.4) / µm	253	339.6
Cold filter plugging point / ºC	-30	-21
Acid number / mg$_{KOH}$ g^{-1}	0.16	0.056
Water content / mg kg^{-1}	60	19.2
Cetane number	58.10	94.8
% C / wt.	85.74	84.68
% H / wt.	14.26	14.525
% O / wt.	0	0
Molecular formula	$C_{13.39}H_{26.72}$	$C_{13.95}H_{28.7}$
Molecular weight	187,4	196.1
Sulfur content / mg kg^{-1}	< 10	<10

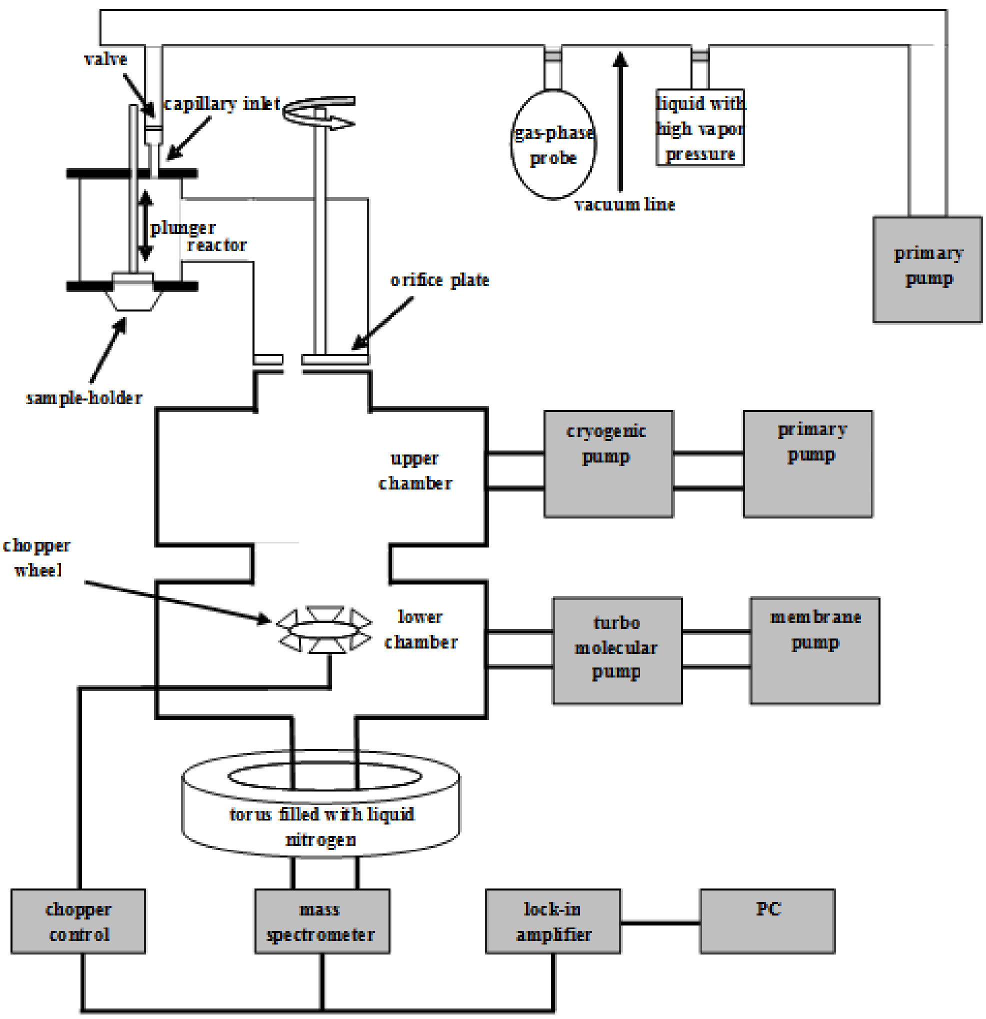

Figure 2S. Schematic drawing of the Knudsen flow reactor.

Table 3S. Knudsen flow reactor parameters for the 1 mm nominal diameter aperture.

Parameter	Value
Volume of the reactor	V = 1830 cm^3
Estimated surface area of the reactor	S = 1300 cm^2
Geometric surface area of the samples	A_s = 10.75 cm^2
Escape orifice diameter	Ø = 1 mm
Chopper frequency	225 Hz
Escape rate constant[a]	$k_{esc} = 0.0058 \sqrt{T/M}\ s^{-1}$

[a] T = temperature/K, M = molecular mass / g mol^{-1}

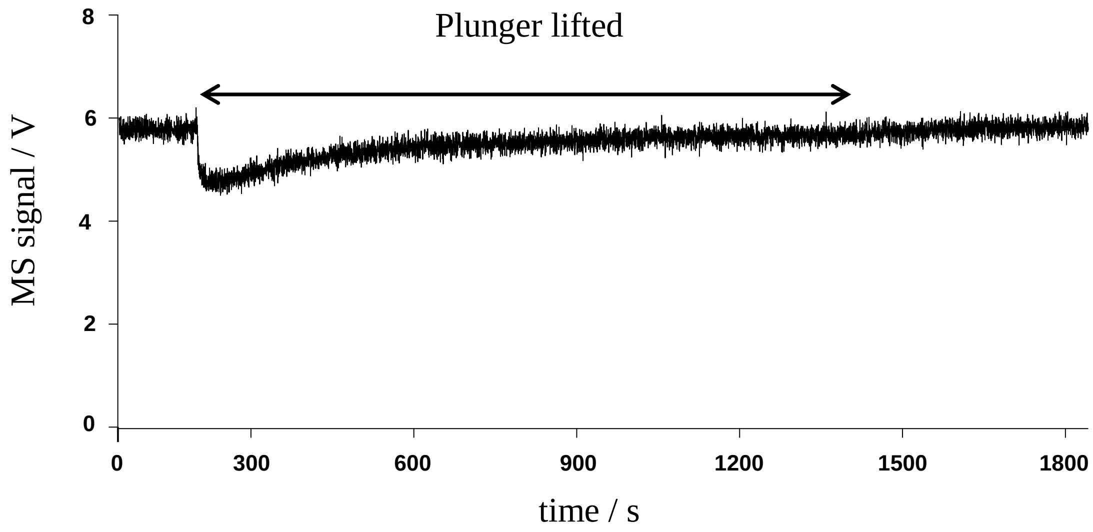

Figure 3S. Raw data of NH_2OH uptake on empty cup at a flow rate of 2.95 × 10^{15} molecule s^{-1} monitored at m/z 33 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0173 s^{-1}).

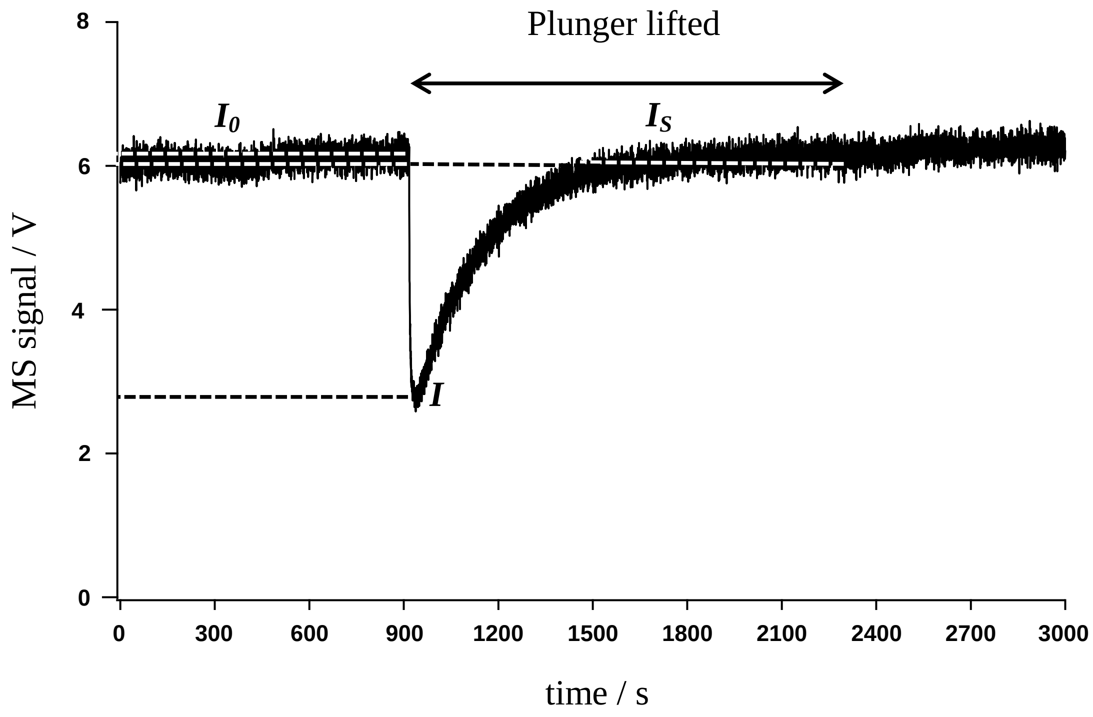

Figure 4S. Raw data of $N(CH_3)_3$ uptake on 16.02 mg PRINTEX XE2-B soot at a flow rate of 3.41×10^{15} molecule s^{-1} monitored at m/z 58 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.013 s^{-1}) leading to the initial uptake coefficient γ_0= 3.37×10^{-4}.

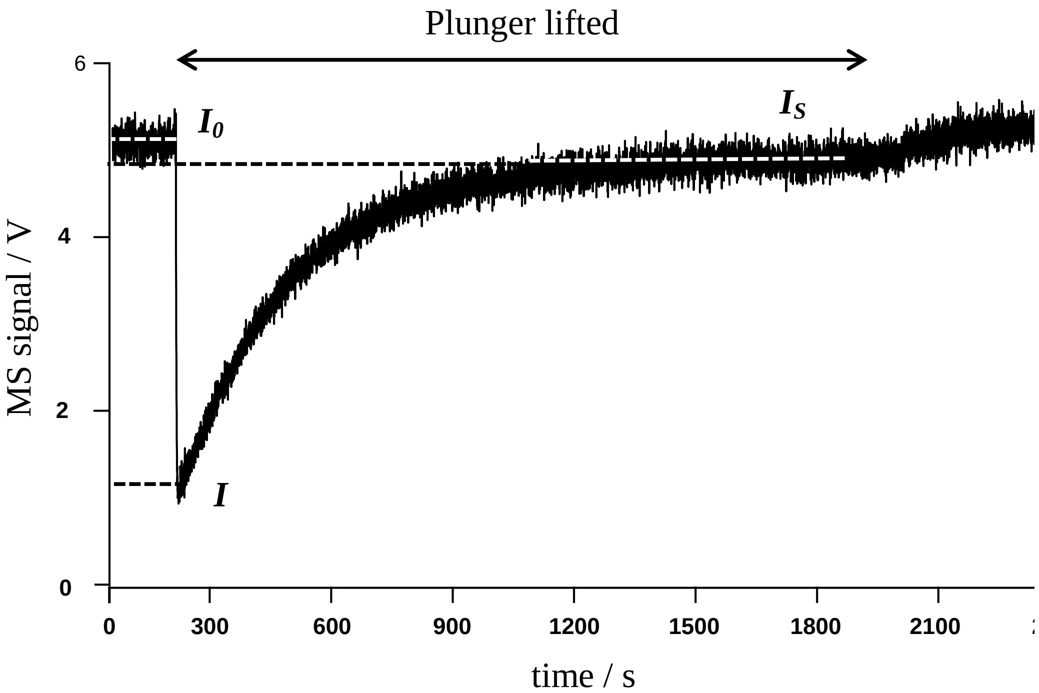

Figure 5S. Raw data of NH_2OH uptake on 20.71 mg Diesel soot at a flow rate of 6.07 × 10^{15} molecule s^{-1} monitored at m/z 33 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0173 s^{-1}) leading to the initial uptake coefficient γ_0= 1.02 × 10^{-3}.

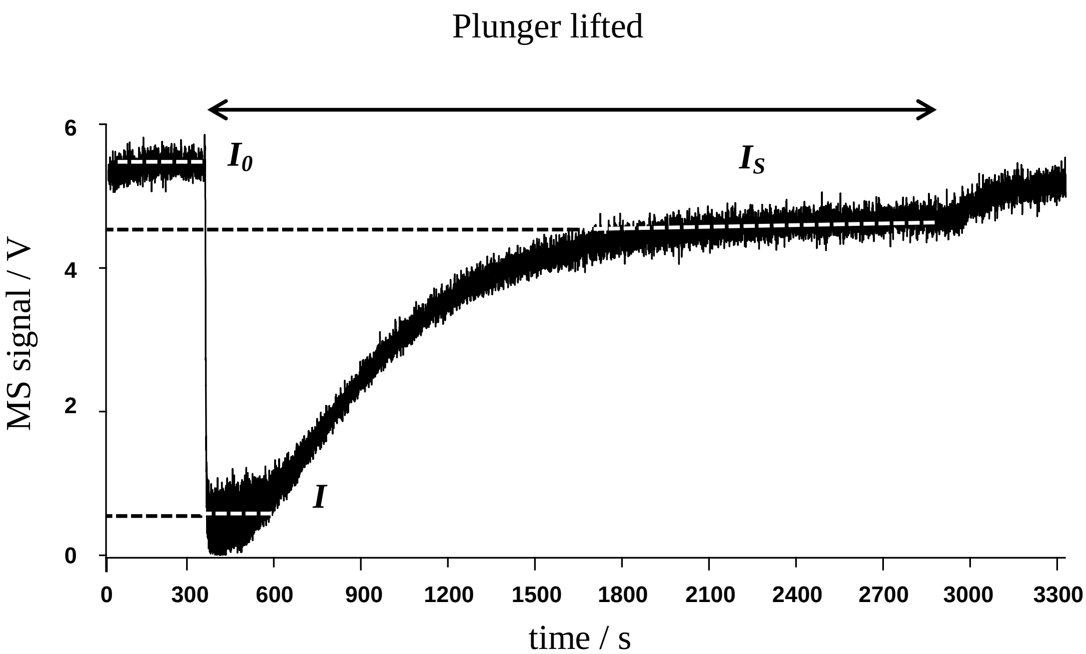

Figure 6S. Raw data of NH_2OH uptake on 16.13 mg HVO soot at a flow rate of 2.90 × 10^{15} molecule s^{-1} monitored at m/z 33 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0173 s^{-1}) leading to the initial uptake coefficient γ_0= 4.40 × 10^{-3}.

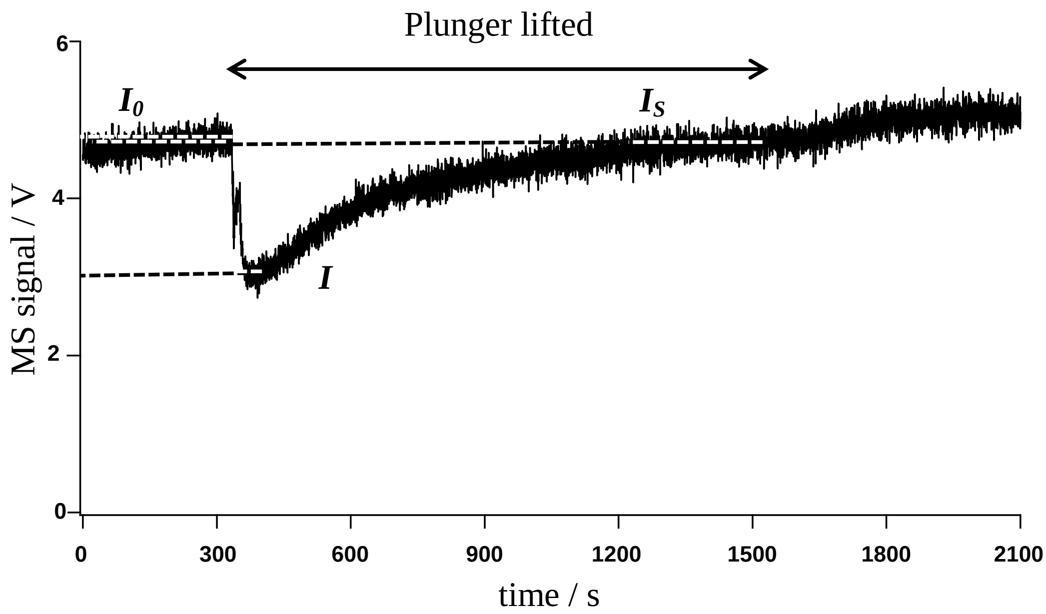

Figure 7S. Raw data of NH_2OH uptake on 10.38 mg PRINTEX XE-B soot at a flow rate of 6.15 × 10^{15} molecule s^{-1} monitored at m/z 33 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0173 s^{-1}) leading to the initial uptake coefficient γ_0= 1.58 × 10^{-4}.

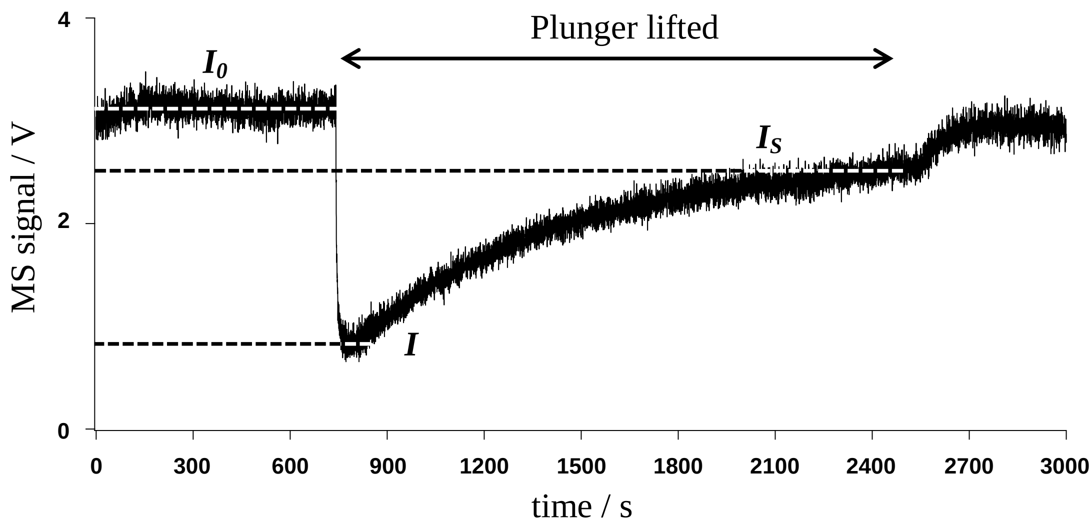

Figure 8S. Raw data of CF_3COOH uptake on 15.15 mg PRINTEX XE-B soot at a flow rate of 2.93 × 10^{15} molecule s^{-1} monitored at m/z 69 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0093 s^{-1}) leading to the initial uptake coefficient γ_0= 7.86 × 10^{-4}.

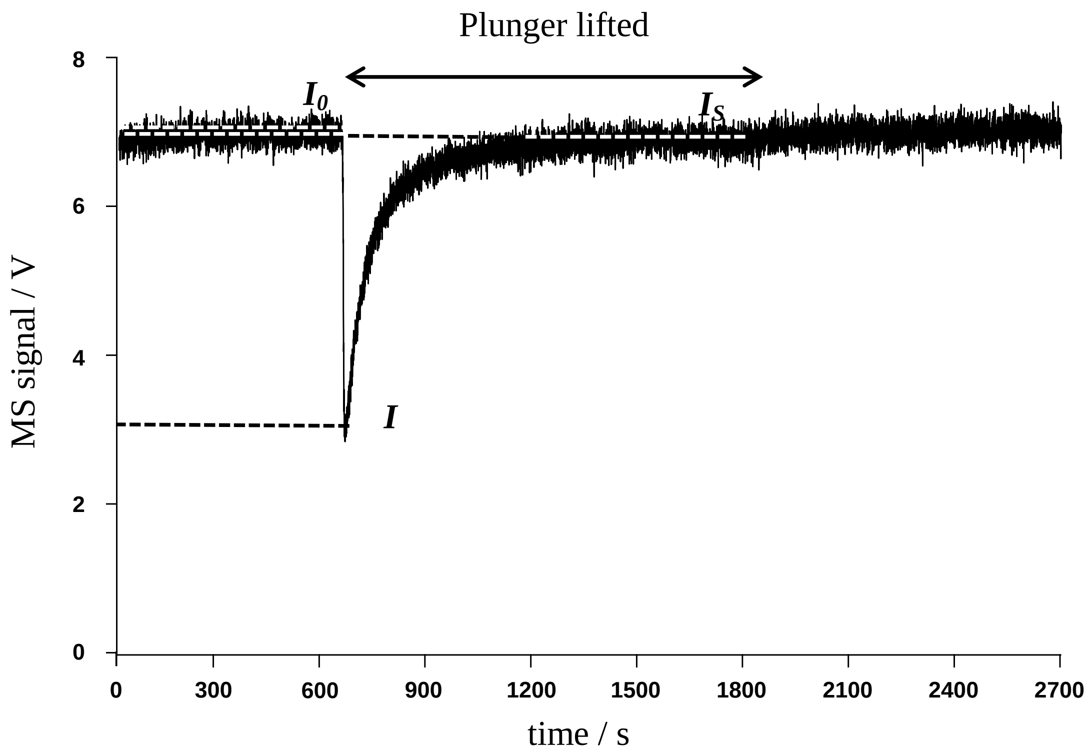

Figure 9S. Raw data of HCl uptake on 10.5 mg Diesel soot at a flow rate of 4.66×10^{15} molecule s^{-1} monitored at m/z 36 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0165 s^{-1}) leading to the initial uptake coefficient γ_0= 3.52×10^{-4}.

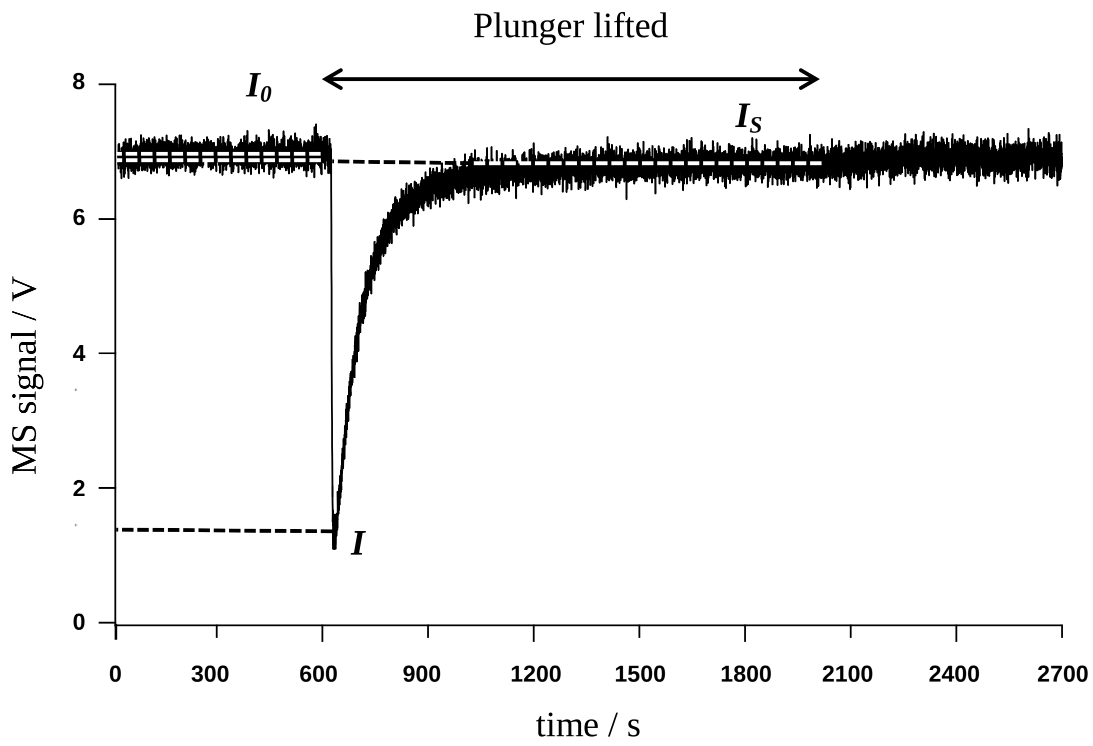

Figure 10S. Raw data of HCl uptake on 10.6 mg HVO soot at a flow rate of 4.48 × 10^{15} molecule s^{-1} monitored at m/z 36 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0165 s^{-1}) leading to the initial uptake coefficient γ_0= 1.25 × 10^{-3}.

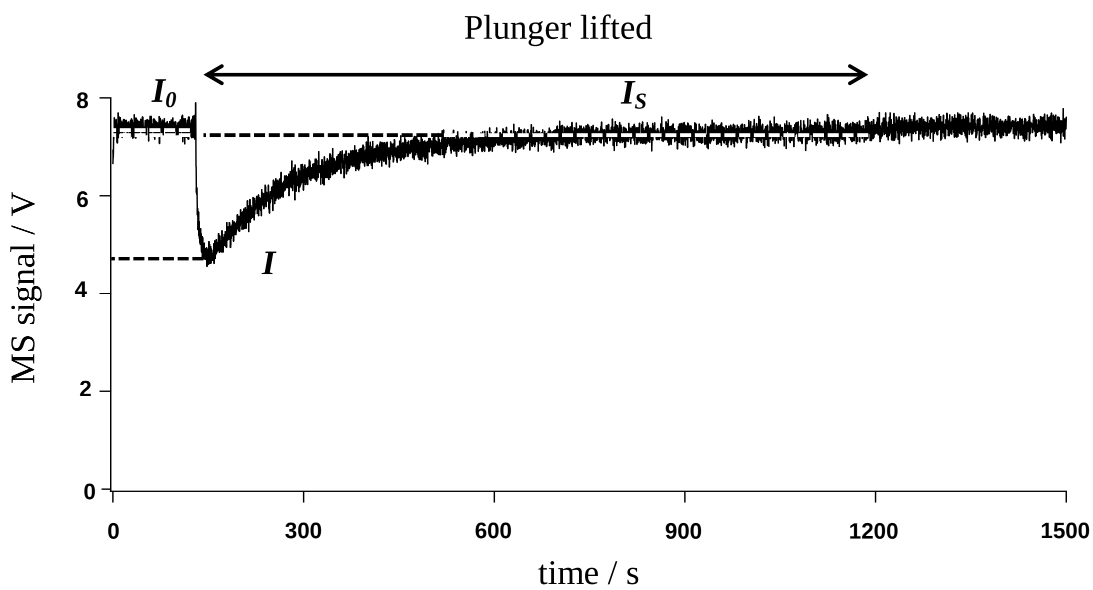

Figure 11S. Raw data of HCl uptake on 15.55 mg PRINTEX XE-B soot at a flow rate of 5.32 × 10^{15} molecule s^{-1} monitored at m/z 36 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0165 s^{-1}) leading to the initial uptake coefficient γ_0= 1.48 × 10^{-4}.

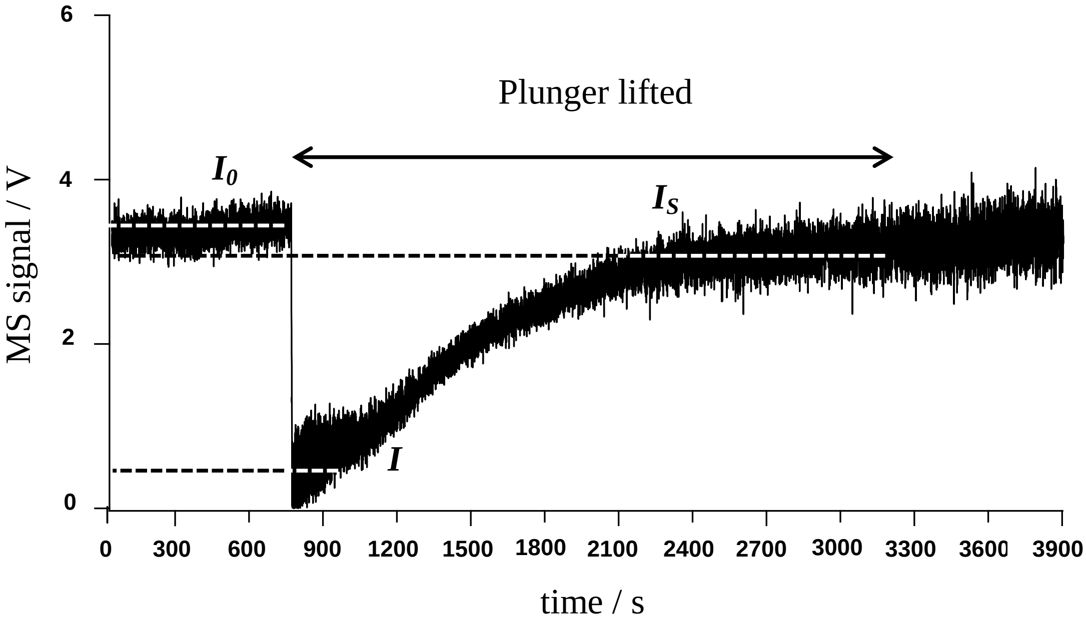

Figure 12S. Raw data of NO_2 uptake on 16.4 mg Diesel soot at a flow rate of 1.13×10^{16} molecule s^{-1} monitored at m/z 46 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.0167 s^{-1}) leading to the initial uptake coefficient γ_0= 3.56×10^{-3}.

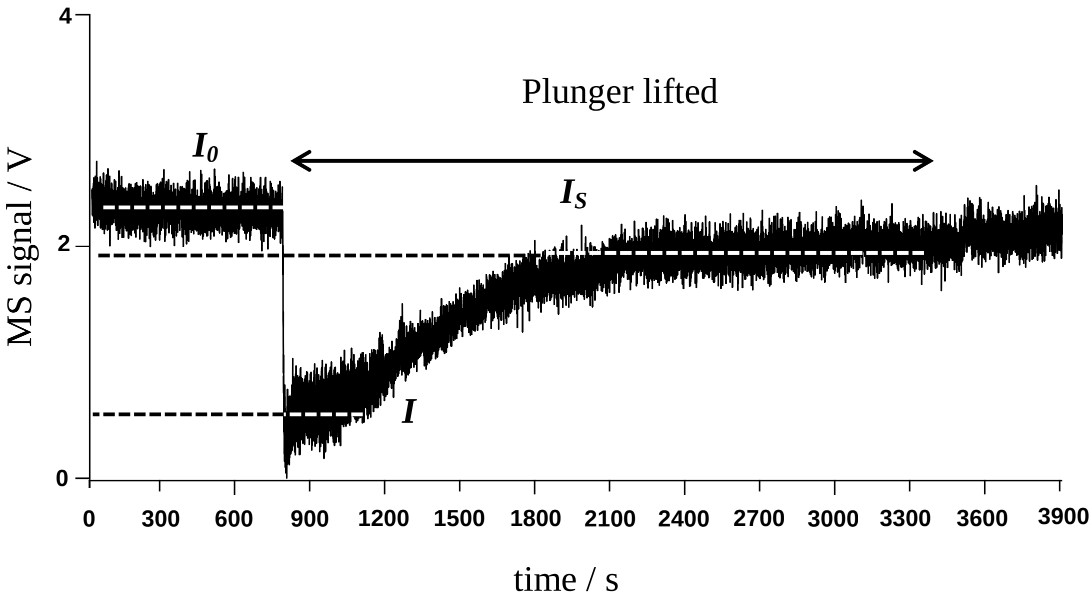

Figure 13S. Raw data of NO_2 uptake on 11.85 mg HVO soot at a flow rate of 8.36×10^{15} molecule s^{-1} monitored at m/z 46 in the 1 mm diameter aperture Knudsen flow reactor (k_{esc}= 0.010 s^{-1}) leading to the initial uptake coefficient γ_0= 6.16×10^{-4}.