

Development of a Portable and Modular Gas Generator: Application to Formaldehyde Analysis

Anaïs Becker¹, Nathaly Lohmann^{1,2}, Christophe A. Serra² and Stéphane Le Calvé^{1,*}

- ¹ Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé, Université de Strasbourg, CNRS, ICPEES UMR 7515, F-67034 Strasbourg, France;
 ana.becker@unistra.fr (A.B.); nathalyloh@gmail.com (N.L.)
- ² Institut Charles Sadron, Université de Strasbourg, CNRS, ICS UPR 22, F-67034 Strasbourg, France; ca.serra@unistra.fr
- * Correspondence: slecalve@unistra.fr

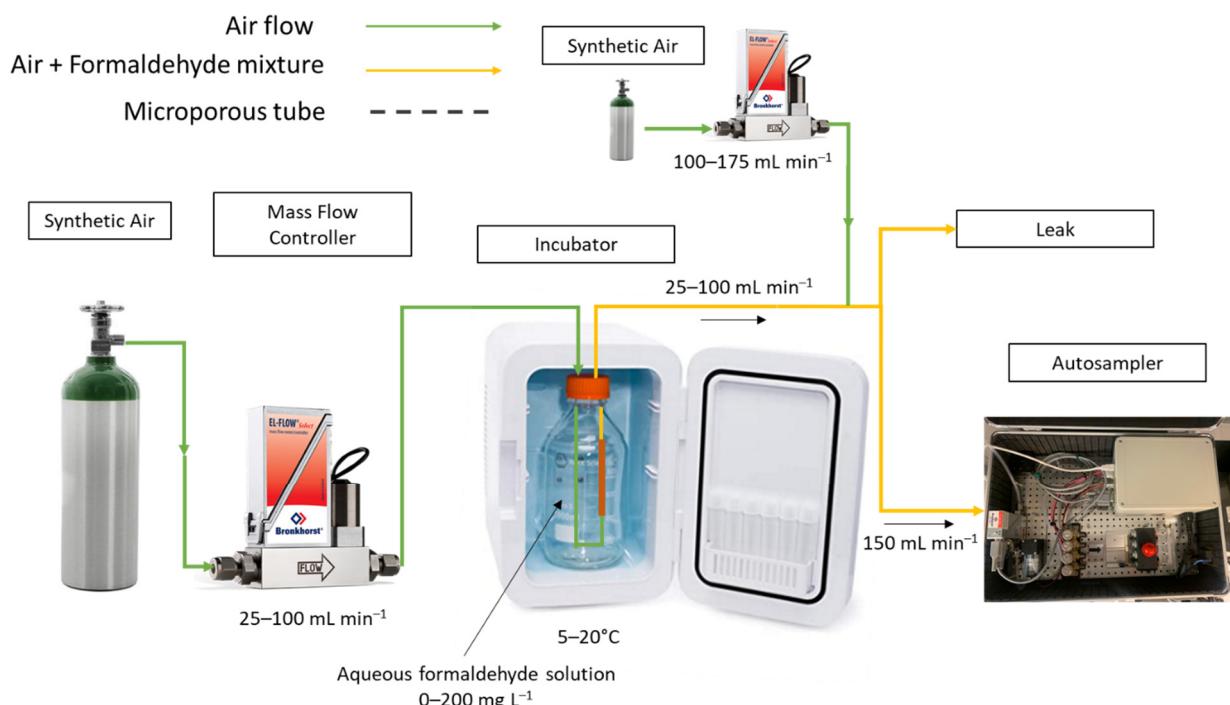


Figure S1. Device used for the generation of gaseous formaldehyde from a liquid solution. This device integrates a cylinder of pure air, a mass flow controller, a glass reactor containing the aqueous formaldehyde solution where the microporous tube and its fixing system are immersed. At the outlet of the device, an autosampler allows a sampling of the gas generated on a DNPH cartridge for a subsequent analysis on HPLC-UV.

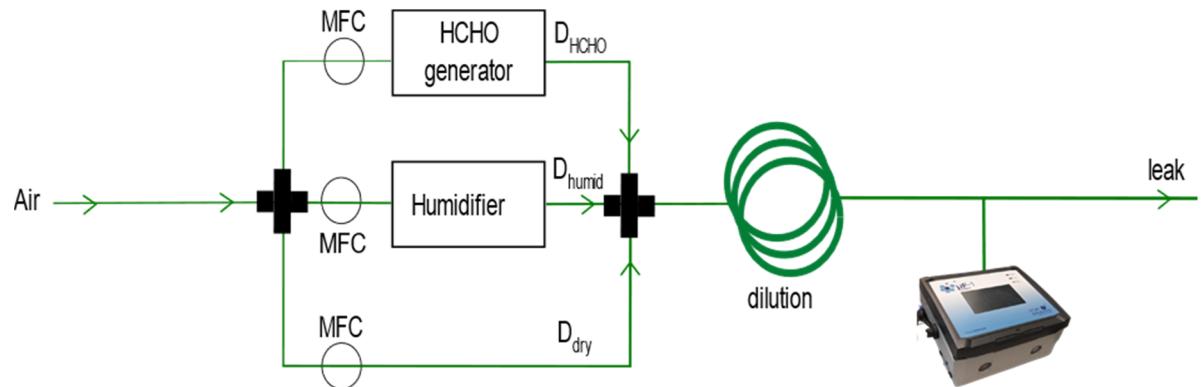


Figure S2. Set-up recommended to vary the relative humidity of a generated gaseous formaldehyde mixture. MFC means Mass Flow Controller. D_{HCHO} , D_{dry} and D_{humid} are the gas flow rates of formaldehyde obtained by developed gas generator, dry air, and humid air, respectively. The humid air is obtained with the same gas generator than that used for formaldehyde, pure water replacing the aqueous formaldehyde solution.

Table S1. Calculation of the autonomy (t_{autonomy}), i.e., the time required for a loss of 1% of the mole number present in the formaldehyde solution at 10,7°C and a gas flow rate F_{gas} of 25, 50 and 100 mL min⁻¹, with a volume of liquid solution of 300 mL and for liquid formaldehyde concentration in the range 2.5–200 mg L⁻¹.

[HCHO] _{liq}	F_{gas}	[HCHO] _{gas}	P_{HCHO}	$n_{\text{HCHO,liq}}$	1% of $n_{\text{HCHO,liq}}$	t_{autonomy}	
mg L ⁻¹	mL min ⁻¹	µg m ⁻³	ppb	Pa	mol	mol	Days
2.5	25	8.56	6.97	7.06×10^{-4}	2.50×10^{-5}	2.50×10^{-7}	23.9
5	25	13.29	10.82	1.10×10^{-3}	4.99×10^{-5}	4.99×10^{-7}	30.8
10	25	28.44	23.16	2.35×10^{-3}	9.99×10^{-5}	9.99×10^{-7}	28.8
20	25	65.31	53.17	5.39×10^{-3}	2.00×10^{-4}	2.00×10^{-6}	25.1
35	25	107.66	87.65	8.88×10^{-3}	3.50×10^{-4}	3.50×10^{-6}	26.7
50	25	153.42	124.91	1.27×10^{-2}	4.99×10^{-4}	4.99×10^{-6}	26.7
100	25	313.99	255.64	2.59×10^{-2}	9.99×10^{-4}	9.99×10^{-6}	26.1
150	25	480.75	391.41	3.97×10^{-2}	1.50×10^{-3}	1.50×10^{-5}	25.6
200	25	682.22	555.44	5.63×10^{-2}	2.00×10^{-3}	2.00×10^{-5}	24.0
2.5	50	2.47	2.01	2.03×10^{-4}	2.50×10^{-5}	2.50×10^{-7}	41.6
5	50	9.84	8.01	8.12×10^{-4}	4.99×10^{-5}	4.99×10^{-7}	20.8
10	50	21.12	17.19	1.74×10^{-3}	9.99×10^{-5}	9.99×10^{-7}	19.4
20	50	44.24	36.02	3.65×10^{-3}	2.00×10^{-4}	2.00×10^{-6}	18.5
35	50	81.10	66.03	6.69×10^{-3}	3.50×10^{-4}	3.50×10^{-6}	17.7
50	50	122.38	99.64	1.01×10^{-2}	4.99×10^{-4}	4.99×10^{-6}	16.7
100	50	236.71	192.72	1.95×10^{-2}	9.99×10^{-4}	9.99×10^{-6}	17.3
150	50	358.75	292.08	2.96×10^{-2}	1.50×10^{-3}	1.50×10^{-5}	17.1
200	50	519.44	422.90	4.29×10^{-2}	2.00×10^{-3}	2.00×10^{-5}	15.8
2.5	100	1.34	1.09	1.10×10^{-4}	2.50×10^{-5}	2.50×10^{-7}	38.3
5	100	6.80	5.53	5.61×10^{-4}	4.99×10^{-5}	4.99×10^{-7}	15.1
10	100	16.79	13.67	1.38×10^{-3}	9.99×10^{-5}	9.99×10^{-7}	12.2
20	100	29.94	24.38	2.47×10^{-3}	2.00×10^{-4}	2.00×10^{-6}	13.7
35	100	52.88	43.05	4.36×10^{-3}	3.50×10^{-4}	3.50×10^{-6}	13.6
50	100	86.59	70.50	7.14×10^{-3}	4.99×10^{-4}	4.99×10^{-6}	11.8
100	100	140.98	114.78	1.16×10^{-2}	9.99×10^{-4}	9.99×10^{-6}	14.5
150	100	223.46	181.93	1.84×10^{-2}	1.50×10^{-3}	1.50×10^{-5}	13.8
200	100	337.44	274.73	2.78×10^{-2}	2.00×10^{-3}	2.00×10^{-5}	12.1

Table S2. Calculation of the theoretical Relative Humidity (RH_{total}) obtained for various conditions and a fixed target formaldehyde concentration of $[\text{HCHO}]_{\text{gas, final}} = 100 \mu\text{g m}^{-3}$ (81.4 ppb) at the outlet of the set-up shown in Figure S2. $T_{\text{HCHO, liq}}$ is the temperature of the liquid solution of formaldehyde; $[\text{HCHO}]_{\text{liq}}$ and $[\text{HCHO}]_{\text{gas}}$ are the formaldehyde concentrations in liquid and gas phases, respectively. The aqueous formaldehyde concentrations have been derived from the linear plots of $[\text{HCHO}]_{\text{gas}}$ vs. $[\text{HCHO}]_{\text{liq}}$. D_{HCHO} , D_{dry} and D_{humid} are the gas flow rates of formaldehyde obtained by developed gas generator, dry air and humid air, respectively. The humid air is obtained with the same gas generator than that used for formaldehyde, pure water replacing the aqueous formaldehyde solution. D_{total} is the resulting total gas flow. RH_{HCHO} , RH_{dry} and RH_{humid} are the experimental relative humidities obtained in this work. RH_{total} is the theoretical resulting final humidity of the gas mixture according to the relative contribution of each gas to the total flow rate.

$T_{\text{HCHO, liq}}$ (°C)	$[\text{HCHO}]_{\text{liq}}$ (mg L ⁻¹)	$[\text{HCHO}]_{\text{gas}}$ ($\mu\text{g m}^{-3}$)	D_{HCHO} (mL min ⁻¹)	D_{dry} (mL min ⁻¹)	D_{humid} (mL min ⁻¹)	D_{total} (mL min ⁻¹)	RH_{HCHO} (%)	RH_{dry} (%)	RH_{humid} (%)	RH_{total} (%)	$[\text{HCHO}]_{\text{gas, final}}$ ($\mu\text{g m}^{-3}$)
10.8	168	400	50	50	100	200	32	3	25	21.3	100.0
10.8	168	400	50	100	50	200	32	3	36	18.5	100.0
10.8	168	400	50	125	25	200	32	3	42	15.1	100.0
10.8	168	400	50	150	0	200	32	3	0	10.3	100.0
10.8	260	800	25	75	100	200	38	3	25	18.4	100.0
10.8	260	800	25	125	50	200	38	3	36	15.6	100.0
10.8	260	800	25	150	25	200	38	3	42	12.3	100.0
10.8	260	800	25	175	0	200	38	3	0	7.4	100.0
21.8	72.5	400	50	50	100	200	49	3	45	35.5	100.0
21.8	72.5	400	50	100	50	200	49	3	57	28.0	100.0
21.8	72.5	400	50	125	25	200	49	3	65	22.3	100.0
21.8	72.5	400	50	150	0	200	49	3	0	14.5	100.0
21.8	97.5	800	25	75	100	200	59	3	45	31.0	100.0
21.8	97.5	800	25	125	50	200	59	3	57	23.5	100.0
21.8	97.5	800	25	150	25	200	59	3	65	17.8	100.0
21.8	97.5	800	25	175	0	200	59	3	0	10.0	100.0
21.8	24.4	200	25	0	25	50	59	3	65	62.0	100.0
21.8	36.6	300	25	0	50	75	59	3	57	57.7	100.0
21.8	61	500	25	0	100	125	59	3	45	47.8	100.0
21.8	27.2	150	50	0	25	75	49	3	65	54.3	100.0
21.8	36.2	200	50	0	50	100	49	3	57	53.0	100.0
21.8	54.3	300	50	0	100	150	49	3	45	46.3	100.0