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Controlled chamber formation of per- and polyfluoroalkyl substances (PFAS) aerosols with *Pseudomonas fluorescens*: size distributions, effects, and inhalation deposition potential

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Table S1 ^{13}C labelled PFAS in the EPA 533 ES isotope dilution standard mix (Wellington laboratories Inc, Canada).

^{13}C labelled PFAS	**Abbreviation**
Perfluorobutanoic acid, $^{13}C_4$	MPFBA
Perfluorobutane sulfonic acid, $^{13}C_3$	M3PFBS
Perfluoropentanoic acid, $^{13}C_5$	M5PFPeA
4:2 fluorotelomer sulfonate, $^{13}C_2$	M2-4:2FTS
Perfluorohexanoic acid, $^{13}C_5$	M5PFHxA
Perfluoroheptanoic acid, $^{13}C_4$	M4PFHpA
Perfluorohexane sulfonic acid, $^{13}C_3$	M3PFHxS
Perflurooctanoic acid, $^{13}C_8$	M8PFOA
6:2 fluorotelomer sulfonate, $^{13}C_2$	M2-6:2FTS
Perfluorononanoic acid, $^{13}C_9$	M9PFNA
Perfluorooctane sulfonic acid, $^{13}C_8$	M8PFOS
Perfluorodecanoic acid, $^{13}C_6$	M6PFDA
8:2 fluorotelomer sulfonate, $^{13}C_2$	M2-8:2-FTS
Perfluoroundecanoic acid, $^{13}C_7$	M7PFUdA
Hexafluoropropylene oxide, $^{13}C_3$	M3HFPO-DA
Perfluorododecanoic acid, $^{13}C_2$	MPFDoA

Table S2. Breathing parameters used in MPPD model (version 2.11, Applied Research Associates, Inc.) to estimate deposition fraction as a function of particle size (Anjilvel and Asgharian, 1995, https://doi.org/10.1006/faat.1995.1144).

Species	Human
Model	Yeh/Schum Symmetric
FRC	3300 ml
URT Volume	50 ml
Breathing frequency	12 /min
Tidal volume	625 ml
Inspiration Fraction	0.5
Pause fraction	0
Body position	Upright
Breathing Scenario	Nasal

Table S3. Regional (head, tracheobronchial region – TB, and Pulmonary/Alveolar Region – Pul) and total deposition efficiencies calculated using MPPD (version 2.11, Applied Research Associates, Inc.) for each nanoMOUDI size bin.

MOUDI stage	13	12	11	10	9	8	7	6	5	4	3	2	1
Particle Size (µm)	0.01–0.018	0.018–0.032	0.032–0.056	0.056–0.1	0.1–0.18	0.18–0.32	0.32–0.56	0.56–1	1–1.8	1.8–3.2	3.2–5.6	5.6–10	10-30
Head	0.1333	0.0825	0.045	0.025	0.0315	0.0235	0.029	0.0537	0.1437	0.2775	0.578	0.886	0.9884
TB	0.406	0.313	0.2105	0.1395	0.092	0.066	0.052	0.0507	0.0555	0.0755	0.0875	0.0605	0.0085
Pul	0.1933	0.2745	0.2855	0.219	0.1415	0.094	0.0755	0.091	0.119	0.1845	0.15	0.037	0.0002
Total	0.7785	0.7066	0.5699	0.4058	0.2825	0.1993	0.179	0.2312	0.3908	0.6557	0.9122	0.9902	0.9998

Table S4. Size segregated deposition flux (pg/h) estimates in the human respiratory tract.

PFAS	Tract region	0.01–0.018	0.018–0.032	0.032–0.056	0.056–0.1	0.1–0.18	0.18–0.32	0.32–0.56	0.56–1	1–1.8	1.8–3.2	3.2–5.6	5.6–10	10-30	Sum	Course (>1.8 um)	Fine (0.1-1.8 um)	UF (<0.1 um)
11 Cl-PF2OUdS	**Head**	0.000	0.000	0.000	0.009	0.082	0.132	0.373	0.143	0.521	0.081	0.029	0.015	0.000	1.384	0.125	1.251	0.009
	TB	0.000	0.000	0.000	0.049	0.238	0.371	0.669	0.135	0.201	0.022	0.004	0.001	0.000	1.691	0.027	1.615	0.049
	AL	0.000	0.000	0.000	0.077	0.366	0.528	0.972	0.243	0.431	0.054	0.007	0.001	0.000	2.679	0.062	2.540	0.077
	Total	0.000	0.000	0.000	0.142	0.731	1.120	2.304	0.616	1.417	0.190	0.045	0.017	0.000	6.583	0.253	6.189	0.142
L-PFBS	**Head**	0.000	0.000	0.000	0.000	0.042	0.082	0.262	0.051	0.146	0.000	0.000	0.000	0.000	0.584	0.000	0.584	0.000
	TB	0.000	0.000	0.000	0.000	0.124	0.232	0.469	0.048	0.056	0.000	0.000	0.000	0.000	0.930	0.000	0.930	0.000
	AL	0.000	0.000	0.000	0.000	0.191	0.330	0.681	0.087	0.121	0.000	0.000	0.000	0.000	1.409	0.000	1.409	0.000
	Total	0.000	0.000	0.000	0.000	0.381	0.700	1.615	0.220	0.397	0.000	0.000	0.000	0.000	3.313	0.000	3.313	0.000
82 FTS	**Head**	0.000	0.000	0.003	0.005	0.064	0.084	0.235	0.076	0.238	0.047	0.103	0.170	0.015	1.039	0.334	0.697	0.008
	TB	0.000	0.000	0.014	0.026	0.188	0.236	0.421	0.071	0.092	0.013	0.016	0.012	0.000	1.088	0.040	1.008	0.040
	AL	0.000	0.000	0.018	0.041	0.288	0.337	0.611	0.128	0.197	0.031	0.027	0.007	0.000	1.687	0.065	1.562	0.060
	Total	0.000	0.000	0.037	0.077	0.576	0.714	1.450	0.325	0.648	0.111	0.162	0.190	0.015	4.304	0.478	3.713	0.113
PFOS	**Head**	5.236	1.234	0.036	0.040	0.076	0.112	0.401	0.098	0.289	0.068	0.213	0.064	0.000	7.867	0.345	0.976	6.546
	TB	15.947	4.682	0.170	0.223	0.222	0.316	0.718	0.093	0.111	0.019	0.032	0.004	0.000	22.538	0.055	1.460	21.023
	AL	7.593	4.106	0.231	0.351	0.341	0.450	1.043	0.167	0.239	0.045	0.055	0.003	0.000	14.623	0.103	2.239	12.280
	Total	30.579	10.570	0.460	0.650	0.681	0.954	2.473	0.423	0.785	0.161	0.336	0.071	0.000	48.143	0.569	5.315	42.259
L-PFHpS	**Head**	0.011	0.001	0.007	0.014	0.078	0.106	0.267	0.104	0.284	0.122	0.147	0.191	0.000	1.332	0.460	0.839	0.033
	TB	0.033	0.003	0.034	0.077	0.226	0.297	0.478	0.099	0.110	0.033	0.022	0.013	0.000	1.425	0.069	1.210	0.147
	AL	0.016	0.003	0.046	0.122	0.348	0.423	0.694	0.177	0.236	0.081	0.038	0.008	0.000	2.191	0.127	1.878	0.185
	Total	0.063	0.007	0.091	0.225	0.695	0.897	1.646	0.449	0.774	0.288	0.232	0.214	0.000	5.581	0.734	4.461	0.386
62 FTS	**Head**	0.071	0.106	0.656	0.213	0.136	0.123	0.738	0.132	0.884	0.235	26.555	3.833	4.687	38.369	35.310	2.013	1.046
	TB	0.216	0.402	3.070	1.190	0.398	0.345	1.324	0.124	0.342	0.064	4.020	0.262	0.040	11.797	4.386	2.533	4.878
	AL	0.103	0.353	4.164	1.868	0.612	0.492	1.922	0.223	0.732	0.156	6.891	0.160	0.001	17.677	7.209	3.981	6.487
	Total	0.414	0.908	8.312	3.461	1.223	1.043	4.556	0.566	2.405	0.555	41.909	4.284	4.741	74.376	51.489	9.793	13.094
PFHxSK(br+Lin)	**Head**	0.006	0.000	0.006	0.011	0.076	0.103	0.277	0.093	0.272	0.112	0.132	0.184	0.000	1.273	0.428	0.821	0.024
	TB	0.017	0.001	0.030	0.063	0.222	0.289	0.497	0.088	0.105	0.031	0.020	0.013	0.000	1.375	0.063	1.201	0.111
	AL	0.008	0.001	0.040	0.099	0.341	0.412	0.722	0.157	0.226	0.075	0.034	0.008	0.000	2.123	0.117	1.857	0.149

	Total	0.032	0.003	0.081	0.184	0.681	0.874	1.711	0.399	0.741	0.265	0.208	0.205	0.000	5.384	0.678	4.405	0.300
L-PFPeS	**Head**	0.000	0.001	0.008	0.014	0.085	0.106	0.275	0.103	0.313	0.156	0.163	0.236	0.000	1.459	0.554	0.882	0.023
	TB	0.000	0.002	0.037	0.080	0.249	0.299	0.493	0.097	0.121	0.042	0.025	0.016	0.000	1.461	0.083	1.258	0.119
	AL	0.000	0.002	0.051	0.125	0.383	0.426	0.715	0.175	0.259	0.103	0.042	0.010	0.000	2.290	0.156	1.957	0.178
	Total	0.000	0.005	0.101	0.232	0.764	0.902	1.696	0.443	0.851	0.368	0.257	0.264	0.000	5.883	0.888	4.657	0.338
42 FTS	**Head**	0.000	0.002	0.007	0.011	0.081	0.119	0.288	0.099	0.298	0.109	0.272	0.079	0.045	1.410	0.505	0.885	0.021
	TB	0.000	0.007	0.035	0.063	0.238	0.334	0.517	0.094	0.115	0.030	0.041	0.005	0.000	1.478	0.077	1.296	0.105
	AL	0.000	0.006	0.047	0.099	0.366	0.475	0.750	0.168	0.246	0.072	0.071	0.003	0.000	2.304	0.146	2.005	0.152
	Total	0.000	0.015	0.094	0.184	0.730	1.007	1.778	0.427	0.809	0.257	0.430	0.088	0.045	5.865	0.820	4.751	0.294
PFBA	**Head**	0.020	0.318	0.023	0.193	0.377	0.585	1.071	1.086	1.847	1.148	1.692	3.423	4.115	15.897	10.378	4.966	0.553
	TB	0.060	1.205	0.106	1.076	1.102	1.642	1.921	1.025	0.714	0.312	0.256	0.234	0.035	9.688	0.838	6.403	2.447
	AL	0.029	1.057	0.143	1.689	1.695	2.338	2.789	1.840	1.530	0.763	0.439	0.143	0.001	14.456	1.346	10.192	2.918
	Total	0.116	2.721	0.286	3.129	3.383	4.958	6.612	4.675	5.024	2.712	2.670	3.825	4.162	44.275	13.370	24.653	6.252
PFDoA	**Head**	0.000	0.003	0.000	0.003	0.010	0.010	0.045	0.036	0.111	0.032	0.015	0.073	0.000	0.340	0.120	0.213	0.007
	TB	0.000	0.012	0.000	0.019	0.031	0.028	0.081	0.034	0.043	0.009	0.002	0.005	0.000	0.264	0.016	0.217	0.031
	AL	0.000	0.011	0.000	0.030	0.047	0.039	0.118	0.062	0.092	0.021	0.004	0.003	0.000	0.427	0.028	0.358	0.041
	Total	0.000	0.027	0.000	0.056	0.094	0.083	0.279	0.157	0.302	0.075	0.023	0.082	0.000	1.180	0.181	0.916	0.083
Cl-PF3ONS	**Head**	0.000	0.000	0.004	0.009	0.079	0.104	0.263	0.104	0.303	0.143	0.186	0.146	0.000	1.342	0.475	0.853	0.014
	TB	0.001	0.000	0.021	0.050	0.230	0.292	0.472	0.098	0.117	0.039	0.028	0.010	0.000	1.358	0.077	1.209	0.072
	AL	0.001	0.000	0.028	0.078	0.354	0.415	0.685	0.176	0.251	0.095	0.048	0.006	0.000	2.138	0.149	1.882	0.107
	Total	0.002	0.000	0.056	0.145	0.706	0.881	1.624	0.448	0.825	0.337	0.294	0.163	0.000	5.482	0.794	4.484	0.203
NaDONA	**Head**	0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.003	0.000	0.000	0.043	0.008	0.021	0.078	0.071	0.007	0.000
	TB	0.000	0.000	0.000	0.000	0.000	0.004	0.005	0.003	0.000	0.000	0.007	0.001	0.000	0.019	0.007	0.011	0.000
	AL	0.000	0.000	0.000	0.000	0.000	0.005	0.007	0.005	0.000	0.000	0.011	0.000	0.000	0.029	0.011	0.017	0.000
	Total	0.000	0.000	0.000	0.000	0.000	0.011	0.017	0.012	0.000	0.000	0.068	0.009	0.021	0.138	0.097	0.040	0.000
GenX	**Head**	0.694	1.001	0.299	0.306	1.015	1.016	1.222	1.719	2.025	2.203	3.408	5.052	1.673	21.633	12.337	6.997	2.300
	TB	2.113	3.796	1.400	1.706	2.963	2.854	2.191	1.623	0.782	0.599	0.516	0.345	0.014	20.904	1.475	10.413	9.016
	AL	1.006	3.329	1.899	2.679	4.558	4.064	3.181	2.914	1.677	1.465	0.885	0.211	0.000	27.868	2.561	16.394	8.913
	Total	4.052	8.570	3.791	4.964	9.100	8.617	7.543	7.402	5.507	5.205	5.379	5.647	1.692	77.468	17.923	38.168	21.377

PFESA	**Head**	0.000	0.000	0.005	0.011	0.074	0.093	0.229	0.090	0.276	0.115	0.116	0.175	0.000	1.184	0.406	0.761	0.017
	TB	0.000	0.000	0.025	0.063	0.215	0.260	0.410	0.085	0.107	0.031	0.018	0.012	0.000	1.226	0.061	1.077	0.088
	AL	0.000	0.000	0.034	0.098	0.331	0.370	0.596	0.153	0.228	0.077	0.030	0.007	0.000	1.925	0.114	1.679	0.133
	Total	0.000	0.000	0.068	0.182	0.660	0.786	1.413	0.389	0.750	0.272	0.183	0.195	0.000	4.899	0.650	3.998	0.251

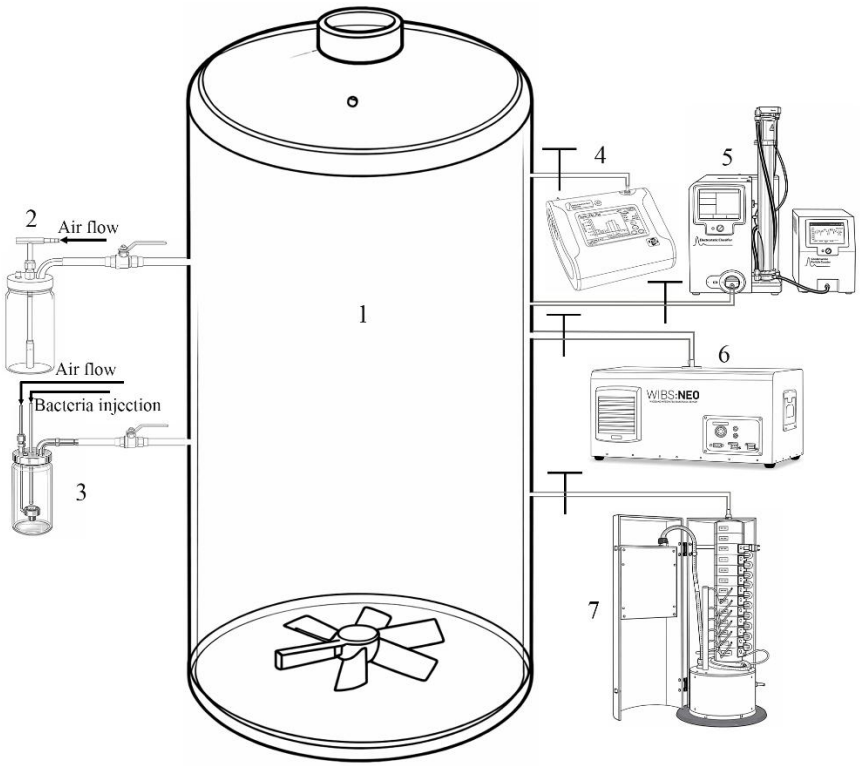

Figure S1. Schematic representation of the experimental setup in the ChAMBRe atmospheric simulation facility. (1) ChAMBRe; (2) three-jet Collison nebuliser used for aerosolisation of the PFAS-containing solution; (3) Sparging Liquid Aerosol Generator (SLAG) used for nebulisation of *Pseudomonas fluorescens*; (4) Optical Particle Sizer (OPS); (5) Scanning Mobility Particle Sizer (SMPS); (6) Waveband Integrated Bioaerosol Sensor (WIBS-NEO); and (7) Nano Micro-Orifice Uniform Deposit Impactor (NanoMOUDI) used for size-resolved aerosol sampling.

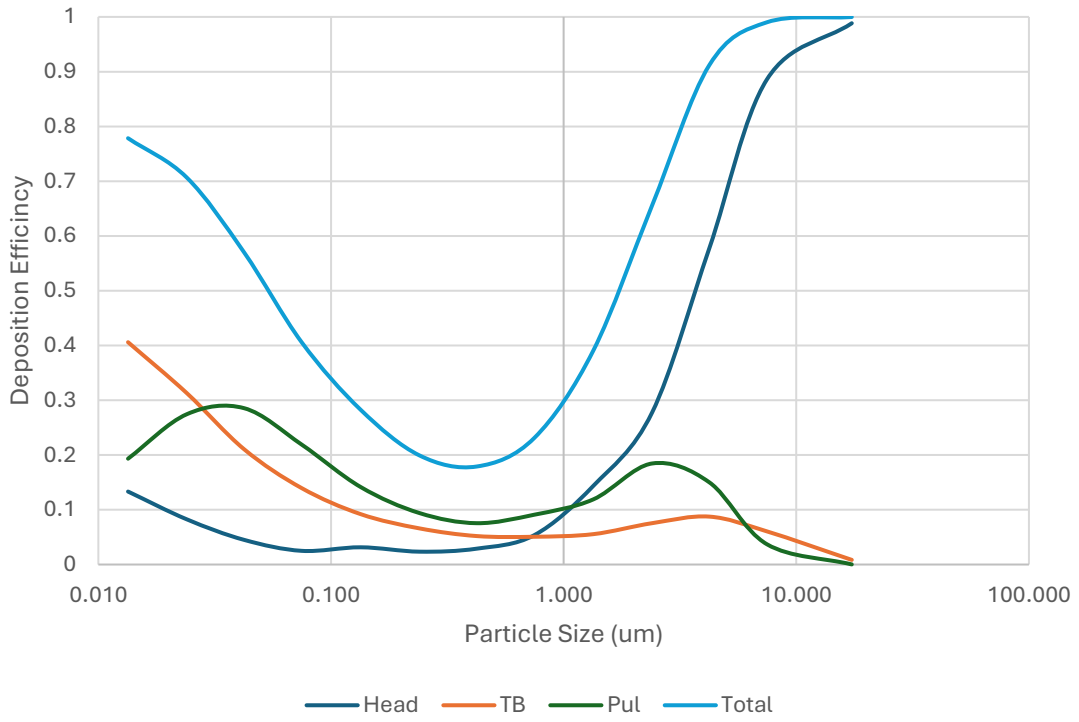

Figure S2. MPPD modelled deposition efficiency in the head, tracheobronchial region, pulmonary region and total human respiratory tract as a function of particle size. MPPD model parameters are given in Table S2.

Chamber dilution correction

Dilution due to aerosol sampling was corrected by accounting for the total sampling flow rate relative to the chamber volume, treating sampling as a first-order loss process. The total volume of ChAMBRe is 2200 L. The connected to the chamber instruments flow was:

- NanoMOUDI 10 L min^{-1};
- TSP: 10 L min^{-1};
- OPS: 1 L min^{-1};
- SMPS: 1 L min^{-1};
- WIBS: 0.3 L min^{-1};

In the experiments with only PFAS, the instruments used were MOUDI, TSP, OPS and SMPS. The dilution factor was 22/2200 min^{-1} = 0.01 min^{-1}.

In the experiments with PFAS + bacteria, the instruments used were MOUDI, TSP, OPS, SMPS and WIBS. The dilution factor was 22.3/2200 min^{-1} = 0.0101 min^{-1}.