Supporting Information

Towards a Universal Model for the Foaming Behavior of Surfactants: A Case Study on Per- and Polyfluoroalkyl Substances (PFAS)

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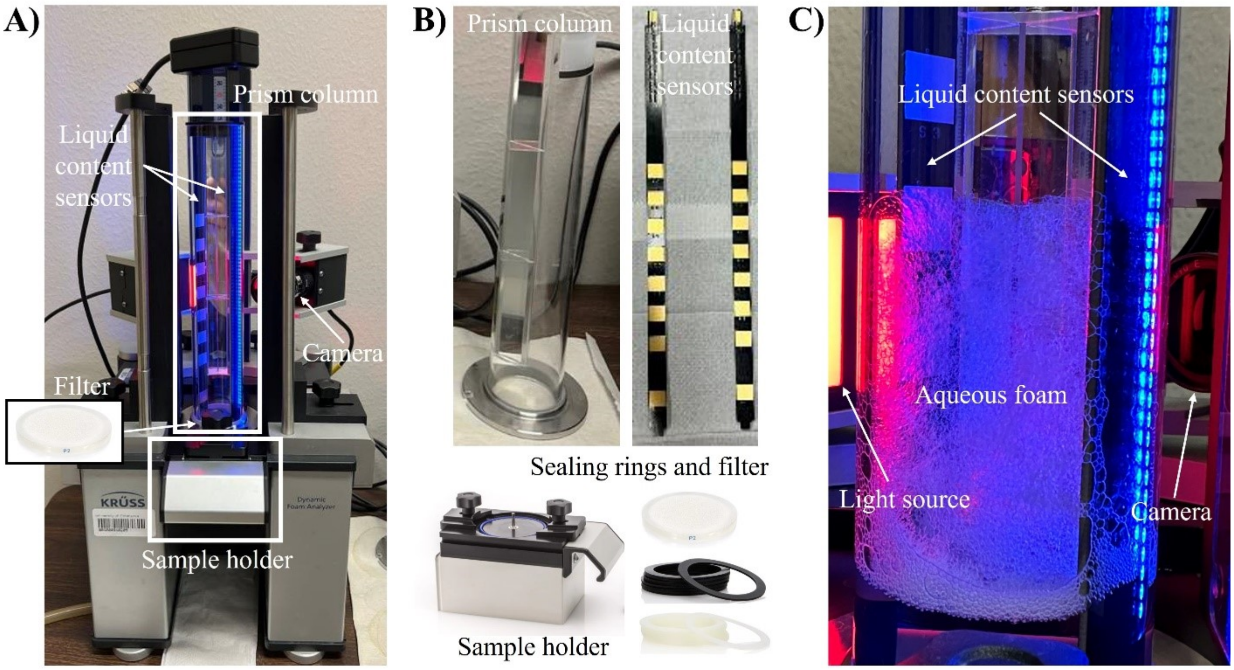

Figure S1. The foam analyzer (*Krüss Scientific, DFA 100*) used in this study: **A)** *DFA 100* setup overview; **B)** details showing the elements of prism column, liquid content sensors, O-rings, glass filter, and sample holder; and **C)** foam sample in the prism column used for morphology observation by using the camera on the back.

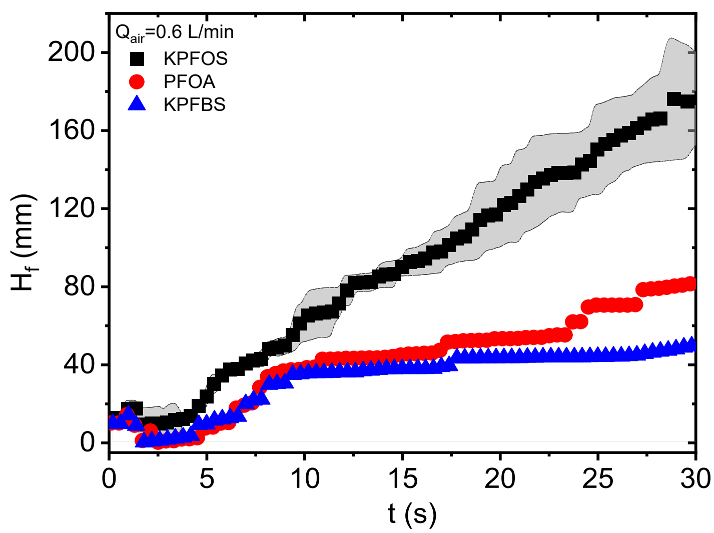

Figure S2. Foam height of 0.4 mM KPFOS, PFOA, and KPFBS aqueous foams during 30 s of aeration. The pore size range of filter was 40-100 μm, and the air flow rate was 0.6 L/min.

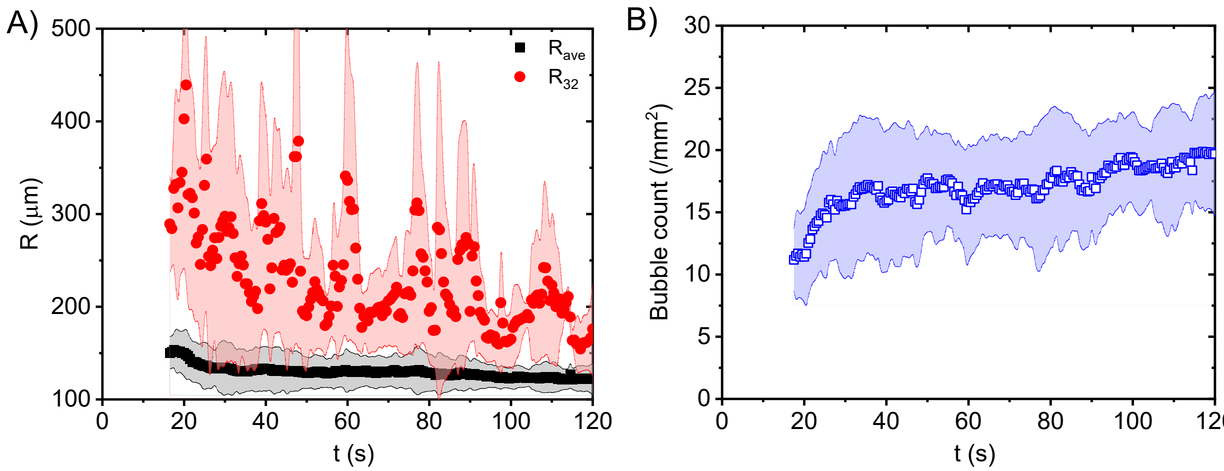

Figure S3. **A)** Average bubble radius including average bubble radius and Sauter mean bubble radius, and **B)** bubble count per area of 0.4 mM KPFOS aqueous foams during foaming process by using 0.2 L/min air flow rate. The filter size was 40-100 μm.

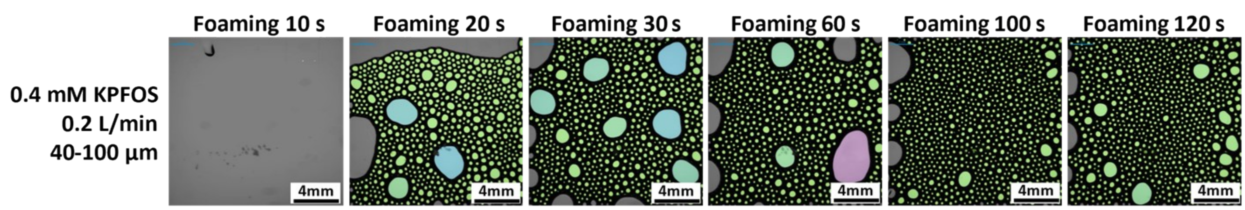

Figure S4. Foam structure at 10, 20, 30, 60, 100 and 120 s during 120 s of foaming for KPFOS at a given bulk concentration of 0.4 mM by using the air flow rate of 0.2 L/min and the glass filter with a pore size range of 40-100 μm. The scale bar is 4 mm.

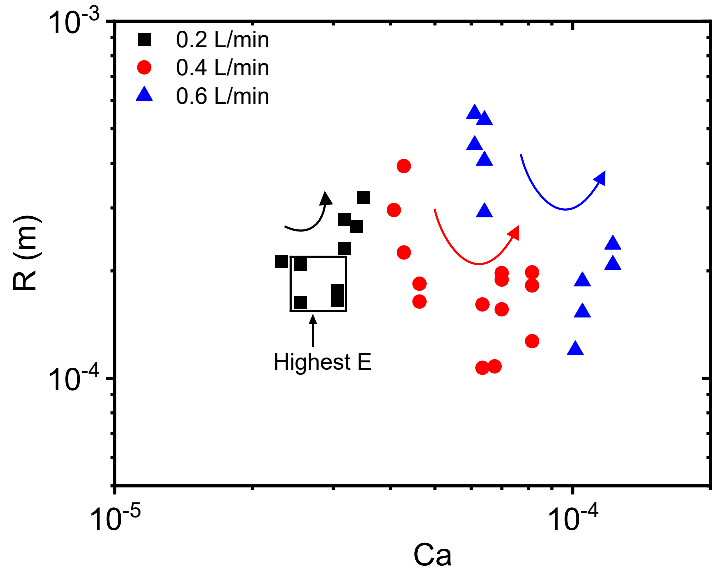

Figure S5. Sauter mean radius of KPFOS aqueous foams with the Capillary number.

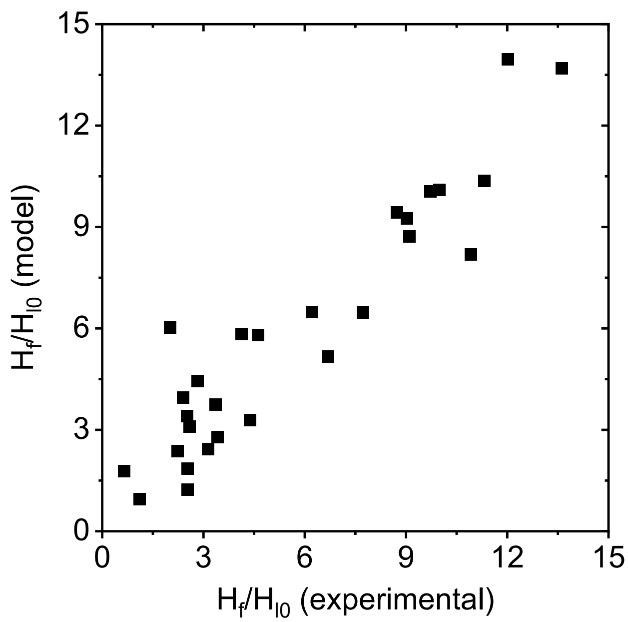

Figure S6. Predicted expansion rate of foaming for KPFOS aqueous solutions by using *Equation (14)*, compared to the experimental expansion rate of foaming for KPFOS aqueous solutions.

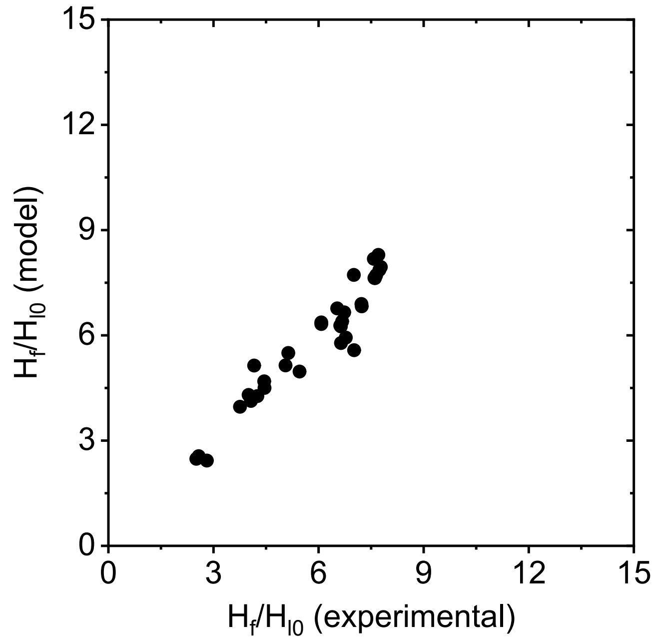

Figure S7. Predicted expansion rate of foaming for PFOA aqueous solutions by using *Equation (15)*, compared to the experimental expansion rate of foaming for PFOA aqueous solutions.

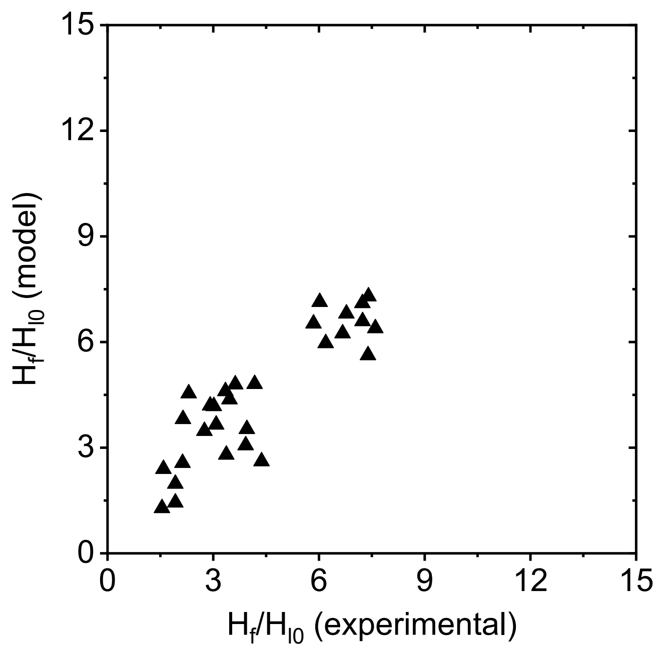

Figure S8. Predicted expansion rate of foaming for KPFBS aqueous solutions by using *Equation (16)* compared to the experimental expansion rate of foaming for KPFBS aqueous solutions.

Table S1. Average bubble radius and Sauter mean bubble radius of KPFOS foams in steady state sparged by using filters with different pore size ranges.

Average bubble radius	
D_f = 40-100 µm	122.33 ± 0.30
D_f = 16-40 µm	84.10 ± 2.37
Sauter mean bubble radius	
D_f = 40-100 µm	162.73 ± 5.34
D_f = 16-40 µm	380.70 ± 109.70

Table S2. Fitted equations for the relationship between the various dimensionless numbers and foaming expansion rate for KPFOS with different bulk concentrations.

Dimensionless number	Q_{air} **(L/min)**	**Equation**	R^2
Re_b	0.2	$\frac{H_f}{H_{l0}} = 0.18612Re_b^{-2.6647}$	0.88308
	0.4	$\frac{H_f}{H_{l0}} = 1.04766Re_b^{-1.9498}$	0.83175
	0.6	$\frac{H_f}{H_{l0}} = 5.35512Re_b^{-1.26729}$	0.96281
Ca	0.2	$\frac{H_f}{H_{l0}} = e^{(-3.36 \times 10^{10}Ca^2 + 1.85 \times 10^6 Ca - 23.7815}$	0.43259
	0.4	$\frac{H_f}{H_{l0}} = e^{(-3.79 \times 10^9 Ca^2 + 4.70 \times 10^5 Ca - 12.5314)}$	0.42501
	0.6	$\frac{H_f}{H_{l0}} = e^{(-1.17 \times 10^9 Ca^2 + 2.29 \times 10^5 Ca - 8.69762)}$	0.90268
We_b	0.2	$\frac{H_f}{H_{l0}} = 2.52 \times 10^{-8} We_b^{-1.64739}$	0.74524
	0.4	$\frac{H_f}{H_{l0}} = 8.90 \times 10^{-10} We_b^{-2.13558}$	0.76102
	0.6	$\frac{H_f}{H_{l0}} = 6.79 \times 10^{-6} We_b^{-1.46065}$	0.75671
Fr_b	0.2	$\frac{H_f}{H_{l0}} = 17169.38Fr_b - 8.88804$	0.78223
	0.4	$\frac{H_f}{H_{l0}} = 2481.44Fr_b - 5.1587$	0.82486
	0.6	$\frac{H_f}{H_{l0}} = 1091.20Fr_b - 1.49395$	0.95948
Bq	0.2	$\frac{H_f}{H_{l0}} = 0.00121Bq - 2.40746$	0.70825
	0.4	$\frac{H_f}{H_{l0}} = 0.00132Bq - 4.00619$	0.87184
	0.6	$\frac{H_f}{H_{l0}} = 0.00156Bq - 1.07306$	0.93758
ζ_p	0.2	$\frac{H_f}{H_{l0}} = -1.508\zeta_p + 1.24257$	0.67863
	0.4		
	0.6		
Θ	0.2	$\frac{H_f}{H_{l0}} = e^{(0.020872\Theta^2 - 2.65715\Theta + 7.99997)}$	0.94397

	0.4	$\frac{H_f}{H_{l0}} = e^{(0.08033\Theta^2 - 1.29406\Theta + 5.72904)}$	0.90474
	0.6	$\frac{H_f}{H_{l0}} = e^{(0.15265\Theta^2 - 2.19106\Theta + 8.98226)}$	0.95009

Table S3. Fitted equations for the relationship between the various dimensionless numbers and foaming expansion rate for 0.4 mM PFOA with different NaCl concentrations.

Dimensionless number	Q_{air} (L/min)	Equation	R^2
Re_b	0.2	$\frac{H_f}{H_{l0}} = 4.01841Re_b - 6.494$	0.96513
	0.4	$\frac{H_f}{H_{l0}} = 10.00765Re_b - 9.24582$	0.7546
	0.6	$\frac{H_f}{H_{l0}} = 8.83394Re_b - 1.86567$	0.96281
Ca	0.2	$\frac{H_f}{H_{l0}} = e^{(-5.57 \times 10^{10}Ca^2 + 2.91 \times 10^6 Ca - 37.1209}$	0.77979
	0.4	$\frac{H_f}{H_{l0}} = e^{(-1.09 \times 10^{10}Ca^2 + 1.11 \times 10^6 Ca - 26.2504}$	0.85435
	0.6	$\frac{H_f}{H_{l0}} = e^{(-1.72 \times 10^9 Ca^2 + 2.71 \times 10^5 Ca - 8.63821)}$	0.77038
We_b	0.2	$\frac{H_f}{H_{l0}} = -1.71 \times 10^5 We_b + 3.58111$	0.93229
	0.4	$\frac{H_f}{H_{l0}} = -1.47 \times 10^5 We_b + 9.12474$	0.73749
	0.6	$\frac{H_f}{H_{l0}} = -1.56 \times 10^4 We_b + 8.37155$	0.60821
Fr_b	0.2	$\frac{H_f}{H_{l0}} = 66.9518Fr_b^{0.0493} - 45.51554$	0.86342
	0.4		
	0.6		
ζ_p	0.2	$\frac{H_f}{H_{l0}} = 0.58829\zeta_p - 0.28905$	0.85787
	0.4		
	0.6		
Θ	0.2	$\frac{H_f}{H_{l0}} = 2.38586\Theta - 5.0019$	0.53985
	0.4	$\frac{H_f}{H_{l0}} = 3.51757\Theta - 1.93135$	0.39088
	0.6	$\frac{H_f}{H_{l0}} = 4.57481\Theta - 2.53595$	0.88125

Table S4. Fitted equations for the relationship between the various dimensionless numbers and foaming expansion rate for 0.4 mM KPFBS with two $CaCl_2$ concentrations.

Dimensionless number	Q_{air} **(L/min)**	**Equation**	R^2
Re_b	0.6	$\frac{H_f}{H_{l0}} = (1.31495 - 0.12052Re_b)^{\frac{1}{0.09908}}$	0.70942
	0.8		
	1.0		
Ca	0.2	$\frac{H_f}{H_{l0}} = e^{(-5.05 \times 10^{10}Ca^2 + 2.14 \times 10^6 Ca - 22.18)}$	0.48255
	0.4	$\frac{H_f}{H_{l0}} = e^{(-7.97 \times 10^{10}Ca^2 + 6.64 \times 10^6 Ca - 136.8464}$	0.54927
	0.6	$\frac{H_f}{H_{l0}} = e^{(-1.25 \times 10^{10}Ca^2 + 1.58 \times 10^6 Ca - 47.98364}$	0.78938
	0.8	$\frac{H_f}{H_{l0}} = e^{(-8.71 \times 10^{9}Ca^2 + 1.48 \times 10^6 Ca - 61.02557)}$	0.63319
	1.0	$\frac{H_f}{H_{l0}} = e^{(-3.30 \times 10^{9}Ca^2 + 6.90 \times 10^5 Ca - 33.80138)}$	0.93183
We_b	0.6	$\frac{H_f}{H_{l0}} = 0.00261We_b^{-0.75396}$	0.49497
	0.8	$\frac{H_f}{H_{l0}} = 3.28 \times 10^{-6}We_b^{-1.51664}$	0.82483
	1.0	$\frac{H_f}{H_{l0}} = 4.19 \times 10^{-4}We_b^{-1.07105}$	0.86344
Fr_b	0.6	$\frac{H_f}{H_{l0}} = 666.54643Fr_b - 0.16715$	0.58216
	0.8	$\frac{H_f}{H_{l0}} = 497.94522Fr_b - 2.4526$	0.76269
	1.0	$\frac{H_f}{H_{l0}} = 352.70274Fr_b - 2.3281$	0.92017
ζ_p	0.2	$\frac{H_f}{H_{l0}} = 0.6598\zeta_p - 0.6121$	0.62076
	0.4		
	0.6		
	0.8		
	1.0		

Table S5. Foaming parameters and experimental values for KPFOS aqueous solutions used for dimensional analysis of foaming expansion rate with $D_c = 0.05\ m$, $D_f = 0.00007\ m$, $\rho = 990\ kg/m^3$, $\eta = 0.001\ kg/s \cdot m$.

KPFOS concentration (ppm)	Q_{air} (m^3/s)	t_e (s)	**Equilibrium?**	γ (N/m)	E (N/m)	η_s ($N \cdot s/m$)	Re_b	Ca	We_b	Fr_b	Bq	Θ	ζ_p	$\frac{R}{H_{l0}}$	$\frac{H_f}{H_{l0}}$
100	3E-06	104.9	Yes	0.0523738	0.013956	0.0018475	0.215	3E-05	5E-06	0.001	11334	4.127	98.01	0.011	10.92
100	3E-06	93.55	Yes	0.0523738	0.013956	0.0018475	0.275	3E-05	7E-06	9E-04	8882	4.127	87.43	0.014	4.379
200	3E-06	95.68	Yes	0.0435405	0.0161413	0.0014776	0.232	3E-05	7E-06	0.001	8396	2.816	89.42	0.012	9.726
200	3E-06	87.96	Yes	0.0435405	0.0161413	0.0014776	0.218	3E-05	7E-06	0.001	8955	2.816	82.2	0.011	11.32
300	3E-06	21.33	Yes	0.0420005	0.0127471	0.0014075	0.305	3E-05	1E-05	8E-04	6093	3.513	19.93	0.015	3.41
300	3E-06	22.73	Yes	0.0420005	0.0127471	0.0014075	0.367	3E-05	1E-05	7E-04	5063	3.513	21.24	0.018	4.902
400	3E-06	13.49	Yes	0.0394964	0.0097478	0.0010724	0.352	3E-05	1E-05	7E-04	4017	4.318	12.61	0.017	2.526
500	3E-06	16.97	Yes	0.0381165	0.0068885	0.0011099	0.425	3E-05	1E-05	6E-04	3447	6.416	15.86	0.021	1.1
10	7E-06	17.78	Yes	0.0623411	0.0078525	0.0010023	0.594	4E-05	3E-05	0.003	4455	8.666	33.23	0.015	2.585
10	7E-06	19.29	Yes	0.0623411	0.0078525	0.0010023	1.038	4E-05	4E-05	0.002	2550	8.666	36.06	0.026	0.648
300	7E-06	39.17	Yes	0.0420005	0.0127471	0.0014075	0.282	6E-05	2E-05	0.007	13154	3.513	73.21	0.007	12.01
300	7E-06	42.46	Yes	0.0420005	0.0127471	0.0014075	0.425	6E-05	3E-05	0.005	8742	3.513	79.36	0.011	8.731
400	7E-06	40.6	Yes	0.0394964	0.0097478	0.0010724	0.285	7E-05	2E-05	0.007	9930	4.318	75.89	0.007	12.41
500	7E-06	22.9	Yes	0.0381165	0.0068885	0.0011099	0.499	7E-05	3E-05	0.004	5873	6.416	42.8	0.012	2.513
500	7E-06	45.47	Yes	0.0381165	0.0068885	0.0011099	0.52	7E-05	4E-05	0.004	5634	6.416	84.99	0.013	2.821
500	7E-06	48.35	Yes	0.0381165	0.0068885	0.0011099	0.412	7E-05	3E-05	0.005	7115	6.416	90.37	0.01	4.13
600	7E-06	17.58	Yes	0.032702	0.0063839	0.001128	0.48	8E-05	4E-05	0.004	6198	6.159	32.86	0.012	3.358
600	7E-06	24.07	Yes	0.032702	0.0063839	0.001128	0.523	8E-05	4E-05	0.004	5697	6.159	44.99	0.013	2.395
600	7E-06	25.57	Yes	0.032702	0.0063839	0.001128	0.335	8E-05	3E-05	0.006	8882	6.159	47.79	0.008	7.73
10	1E-05	16.87	Yes	0.0623411	0.0078525	0.0010023	1.156	6E-05	7E-05	0.006	3433	8.666	47.3	0.019	4.385
10	1E-05	18.88	Yes	0.0623411	0.0078525	0.0010023	2.095	6E-05	1E-04	0.003	1895	8.666	52.93	0.035	2.526
10	1E-05	18.7	Yes	0.0623411	0.0078525	0.0010023	1.612	6E-05	1E-04	0.004	2463	8.666	52.43	0.027	3.135
400	1E-05	34.71	Yes	0.0394964	0.0097478	0.0010724	0.475	1E-04	5E-05	0.014	8937	4.318	97.32	0.008	13.61
500	1E-05	48.05	Yes	0.0381165	0.0068885	0.0011099	0.741	1E-04	8E-05	0.009	5935	6.416	134.7	0.012	9.098
500	1E-05	41.8	Yes	0.0381165	0.0068885	0.0011099	0.606	1E-04	6E-05	0.011	7254	6.416	117.2	0.01	9.988

600	1E-05	17.67	Yes	0.032702	0.0063839	0.001128	0.824	1E-04	1E-04	0.008	5423	6.159	49.54	0.014	6.211
600	1E-05	14.47	Yes	0.032702	0.0063839	0.001128	0.939	1E-04	1E-04	0.007	4760	6.159	40.57	0.016	6.682
600	1E-05	18.65	Yes	0.032702	0.0063839	0.001128	0.939	1E-04	1E-04	0.007	4760	6.159	52.29	0.016	4.614

Table S6. Foaming parameters and experimental values for 0.4 mM PFOA aqueous solutions containing varied concentrations of NaCl used for dimensional analysis of foaming expansion rate with $D_c = 0.05\ m$, $D_f = 0.00007\ m$, $\rho = 990\ kg/m^3$, $\eta = 0.001\ kg/s \cdot m$.

NaCl concentration (mM)	Q_{air} (m^3/s)	t_e (s)	**Equilibrium?**	γ (N/m)	E (N/m)	η_s ($N \cdot s/m$)	Re_b	Ca	We_b	Fr_b	Bq	Θ	ζ_p	$\frac{R}{H_{l0}}$	$\frac{H_f}{H_{l0}}$
10	3E-06	11.85	Yes	0.054358	0.003888	0.000627	0.18744	2.45E-05	4.6E-06	0.001277	4416.146	13.98273	11.07447	0.009294	2.814343
50	3E-06	20.38	Yes	0.051833	0.004609	0.00075	0.21648	2.57E-05	5.57E-06	0.001105	4571.279	11.24561	19.04622	0.010734	2.578724
100	3E-06	20.51	Yes	0.049115	0.003541	0.000638	0.23496	2.71E-05	6.38E-06	0.001018	3582.166	13.8722	19.16771	0.01165	2.513274
0	7E-06	14.32	Yes	0.052562	0.009497	0.00086	0.5808	5.07E-05	2.95E-05	0.003296	3906.82	5.534512	26.76564	0.014399	3.756821
0	7E-06	18.1	Yes	0.052562	0.009497	0.00086	0.528	5.07E-05	2.68E-05	0.003626	4297.502	5.534512	33.83087	0.01309	4.25424
0.5	7E-06	13.09	Yes	0.057208	0.008201	0.000947	0.6468	4.66E-05	3.01E-05	0.00296	3864.334	6.976007	24.46664	0.016035	4.07098
0.5	7E-06	20.67	Yes	0.057208	0.008201	0.000947	0.48048	4.66E-05	2.24E-05	0.003984	5201.988	6.976007	38.63448	0.011912	4.457135
0.5	7E-06	19.06	Yes	0.057208	0.008201	0.000947	0.60456	4.66E-05	2.82E-05	0.003167	4134.331	6.976007	35.62522	0.014988	4.457135
1	7E-06	50.29	Yes	0.056617	0.007263	0.001171	0.48576	4.71E-05	2.29E-05	0.003941	6364.537	7.79571	93.9975	0.012043	6.080291
1	7E-06	54.76	Yes	0.056617	0.007263	0.001171	0.52272	4.71E-05	2.46E-05	0.003662	5914.519	7.79571	102.3524	0.012959	6.636614
5	7E-06	38.71	Yes	0.056704	0.005839	0.000771	0.3432	4.7E-05	1.61E-05	0.005578	5929.746	9.711208	72.35321	0.008508	5.622142
5	7E-06	45.56	Yes	0.056704	0.005839	0.000771	0.36168	4.7E-05	1.7E-05	0.005293	5626.766	9.711208	85.15661	0.008967	5.078908
10	7E-06	25.76	Yes	0.054358	0.003888	0.000627	0.35112	4.91E-05	1.72E-05	0.005452	4714.983	13.98273	48.14825	0.008705	6.780604
10	7E-06	36.6	Yes	0.054358	0.003888	0.000627	0.43824	4.91E-05	2.15E-05	0.004368	3777.667	13.98273	68.40939	0.010865	6.643159
10	7E-06	53.45	Yes	0.054358	0.003888	0.000627	0.41712	4.91E-05	2.05E-05	0.004589	3968.942	13.98273	99.90388	0.010341	6.636614
50	7E-06	45.74	Yes	0.051833	0.004609	0.00075	0.34056	5.14E-05	1.75E-05	0.005621	5811.549	11.24561	85.49305	0.008443	6.734789
100	7E-06	25.6	Yes	0.049115	0.003541	0.000638	0.51744	5.43E-05	2.81E-05	0.0037	3253.192	13.8722	47.84919	0.012828	5.059273
100	7E-06	37.55	Yes	0.049115	0.003541	0.000638	0.50952	5.43E-05	2.77E-05	0.003757	3303.76	13.8722	70.18505	0.012632	5.137813
200	7E-06	17.07	Yes	0.046207	0.00411	0.000744	0.55704	5.77E-05	3.21E-05	0.003437	3526.18	11.24333	31.90569	0.01381	4.45059
200	7E-06	40.52	Yes	0.046207	0.00411	0.000744	0.63096	5.77E-05	3.64E-05	0.003034	3113.071	11.24333	75.7363	0.015643	4.16261

200	7E-06	15.54	Yes	0.046207	0.00411	0.000744	0.6732	5.77E-05	3.89E-05	0.002844	2917.741	11.24333	29.04596	0.01669	4.005531
0	1E-05	29.89	Yes	0.052562	0.009497	0.00086	1.15632	7.61E-05	8.8E-05	0.005587	2943.494	5.534512	83.80151	0.019111	7.016224
0.5	1E-05	23.7	Yes	0.057208	0.008201	0.000947	1.01376	6.99E-05	7.09E-05	0.006373	3698.288	6.976007	66.44683	0.016755	6.675884
0.5	1E-05	28.72	Yes	0.057208	0.008201	0.000947	0.94644	6.99E-05	6.62E-05	0.006827	3961.347	6.976007	80.52122	0.015643	6.531895
1	1E-05	36.35	Yes	0.056617	0.007263	0.001171	0.83952	7.06E-05	5.93E-05	0.007696	5523.938	7.79571	101.9132	0.013875	7.579092
1	1E-05	30.72	Yes	0.056617	0.007263	0.001171	0.9108	7.06E-05	6.43E-05	0.007094	5091.63	7.79571	86.12855	0.015053	7.009679
5	1E-05	16.28	Yes	0.056704	0.005839	0.000771	0.54648	7.05E-05	3.85E-05	0.011823	5585.993	9.711208	45.64364	0.009032	7.297658
5	1E-05	22.47	Yes	0.056704	0.005839	0.000771	0.82368	7.05E-05	5.81E-05	0.007844	3706.091	9.711208	62.99832	0.013614	7.225663
5	1E-05	24.65	Yes	0.056704	0.005839	0.000771	0.58608	7.05E-05	4.13E-05	0.011024	5208.561	9.711208	69.11031	0.009687	6.780604
10	1E-05	33.55	Yes	0.054358	0.003888	0.000627	0.693	7.36E-05	5.1E-05	0.009323	3583.387	13.98273	94.06291	0.011454	7.736172
10	1E-05	33.16	Yes	0.054358	0.003888	0.000627	0.59796	7.36E-05	4.4E-05	0.010805	4152.932	13.98273	92.96949	0.009883	7.101308
50	1E-05	41.59	Yes	0.051833	0.004609	0.00075	0.80784	7.72E-05	6.23E-05	0.007998	3674.95	11.24561	116.6044	0.013352	7.611817
100	1E-05	36.97	Yes	0.049115	0.003541	0.000638	0.68508	8.14E-05	5.58E-05	0.009431	3685.697	13.8722	103.6514	0.011323	7.644542
200	1E-05	33.53	Yes	0.046207	0.00411	0.000744	0.83952	8.66E-05	7.27E-05	0.007696	3509.547	11.24333	94.00684	0.013875	7.232208

Table S7. Summary table for the universal equations of KPFOS, PFOA, and KPFBS aqueous foams.

PFAS	Monomial form	R^2
KPFOS	$\frac{H_f}{H_{l0}} = 1587.63 \cdot Re_b^{-1.72} \cdot e^{\left(-9.00 \times 10^7 \cdot Ca^2 + 2.00 \times 10^4 \cdot Ca\right)} \cdot We_b^{-0.44} \cdot Fr_b^{1.02} \cdot Bq^{0.72} \cdot e^{\left(0.097 \cdot \Theta^2 - 1.07 \cdot \Theta\right)} \cdot \zeta_p^{0.45} \cdot (\frac{R}{H_{l0}})^{2.85}$	0.86605
PFOA	$\frac{H_f}{H_{l0}} = 3.06 \cdot e^{\left(-1.00 \times 10^8 \cdot Ca^2 + 1.00 \times 10^4 \cdot Ca\right)} \cdot Fr_b^{0.41} \cdot Bq^{0.38} \cdot \Theta^{0.26} \cdot \zeta_p^{0.16} \cdot (\frac{R}{H_{l0}})^{0.42}$	0.96797
KPFBS	$\frac{H_f}{H_{l0}} = 12.30 * e^{\left(-4.00 \times 10^7 * Ca^2\right)} * Fr_b^{0.51} * \zeta_p^{0.37}$	0.73937

Determining fitting coefficients in dimensional analysis

Generally, the *Equations (9)* can be rewritten to a monomial form as shown below to predict the foaming behavior, herein foaming expansion rate:

$$\frac{H_f}{H_{l0}} = C_0 * Re_b^a * Ca^b * We_b^c * Fr_b^d * Bq^e * \Theta^f * \zeta_p^g * (\frac{R}{H_{l0}})^h * (\frac{D_c}{H_{l0}})^i * (\frac{D_f}{H_{l0}})^j$$ Equation (S1)

where C_0, a, b, c, d, e, f, g, h, and i are constants need to be fitted.

In this work, the Solver function in Excel spreadsheet is used to obtain the as-mentioned coefficients. The *Equation (S1)* is taken the natural logarithm to linearize the equation prior to applying the Solver function. 0.5 is used as the initial guess for all coefficients. The *Equation (S2)* shown below is set as the objective which needs to be the smallest in the Solver function to obtain the coefficients.

$$O = \frac{\sum_{i=1}^{n} \sqrt{|y_i - \hat{y}_i|}}{n}$$ *Equation (S2)*

where y_i is the observed value, $\hat{y}_i$ is the predicted value, n is the sample size. In some cases, the coefficients need to be manually adjusted to obtain the relatively small O for the prediction after the first run of Solver function by using 0.5 as the initial values. Once the coefficients are obtained, the predicted values vs the experimental values are plotted to verify the goodness of fitting. To further determine how well the model fits the data, the R^2 of the model fitting is calculated according to the equations below:

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - a_0 - a_1 m_i - a_2 n_i - \dots - a_j p_i)$$ *Equation (S3a)*

$$S_r = \sum_{i=1}^{n} (e_i)^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 m_i - a_2 n_i - \dots - a_j p_i)^2$$ *Equation (S3b)*

$$S_t = \sum_{i=1}^{n} (y_i - \bar{y})^2$$ *Equation (S3c)*

$$R^2 = \frac{S_t - S_r}{S_t}$$ *Equation (S3d)*

where e_i is the error or called residual, a_i is the coefficients, m_i, n_i, …, p_i are the independent variables, S_r is the residual sum of squares, S_t is the total sum of squares, $\bar{y}$ is the mean of the experimental values, R^2 is the coefficient of determination.