Supporting Information for:

Predicting Pyrolysis Decomposition of PFOA using Computational Nanoreactors: A Thermodynamic Study

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Temperature (K)	k_{push}	α	Observations
298.15	0.04	0.7	Sporadic movement
1000	0.04	0.7	Sporadic movement with occasional bond breakage and reformation
1000	0.05	0.7	Sporadic movement with occasional bond breakage and reformation Rotation from carboxyl group
1300	0.04	0.7	Sporadic movement
1300	0.08	0.7	Sporadic movement with occasional bond breakage and reformation
1300	0.08	0.7	Sporadic movement with occasional bond breakage and reformation
1300	0.12	0.7	Sporadic movement with occasional bond breakage and reformation The hydrogen interacted with the fluorine's
1300	0.2	0.7	The molecule curls onto itself. The carboxyl group disconnects more often, and the hydrogen interacts with the fluorine
1300	0.4	0.7	Simulation failure

Table S1. Observations with change in k_{push}.

Table S2. Observations with change in α.

Temperature (K)	k_{push}	α	Observations
1300	0.2	1	Sporadic movement with occasional bond breakage and reformation
1300	0.2	1.2	Sporadic movement with occasional bond breakage and reformation
1300	0.2	1.4	Sporadic movement with occasional bond breakage and reformation
1300	0.2	1.6	Sporadic movement with occasional bond breakage and reformation

Table S3. Observations of change of k_{push} and alpha.

Temperature (K)	k_{push}	α	Observations
1300	0.3	1.4	Sporadic movement with occasional bond breakage and reformation
1300	0.4	1.4	$C_3F_4O_2H$ broke off and separated into CO_2H and C_2F_4 Resulted in simulation failure
1300	0.5	1.4	Simulation failure
1300	0.5	1.6	CO_2 broke off, the hydrogen first attached to a F and then the carbon creating $C_7F_{15}H$
1300	0.4	1.6	CO_2 and HF broke off

Table S4. Observations of the decomposition species within the nanoreactor.

Species	Temperature (K)	k_{push}	α	Observations
$C_8F_{15}O_2H$	1300	0.4	1.6	Split into CO_2 and C_2F_4
C_7F_{14}	1300	0.4	1.6	Temporarily split into C_3F_5 and C_4F_9 and reformed into C_7F_{14} Split into CF_3 and C_6F_{11}
C_6F_{11}	1300	0.4	1.6	C_2F_4 detached within the first few moments and there is C_4F_7
C_4F_7	1300	0.4	1.6	Simulation failure
	1300	0.4	1.9	Simulation failure
	1300	0.4	2.2	Simulation failure
	1300	0.4	1.6	Simulation failure
	1300	0.2	1.6	Split into C_2F_3 and C_2F_4
C_2F_4	1300	0.2	1.6	Splits into 2 CF_2 and reformed into C_2F_4 and shortly after resulting in a simulation failure

Table S5. Total ΔG values (kJ•mol^{-1}) of the reaction at different temperatures.

Temperature (K)	$C_8F_{15}O_2H$	$C_7F_{14} + CO_2 + HF$	$C_6F_{11} + CF_3 + HF + CO_2$	$C_4F_7 + C_2F_4 + CF_3 + CO_2 + HF$	$C_2F_3 + 2\ C_2F_4 + CF_3 + CO_2 + HF$
298	0	186.44	287.23	397.56	580.66
398	0	150.96	232.04	320.95	484.59
498	0	115.31	176.73	244.30	388.48
598	0	79.66	121.59	167.86	292.63
698	0	44.10	66.69	91.71	197.15
798	0	8.70	12.01	15.94	102.09
898	0	-26.53	-42.38	-59.50	7.45
998	0	-61.63	-96.52	-134.56	-86.73
1098	0	-96.52	-150.41	-209.24	-180.54
1198	0	-131.29	-204.10	-283.68	-273.93
1298	0	-165.90	-257.48	-357.77	-366.94

Table S6. Total ΔG values (kJ•mol^{-1}) of the recombination of CF_3 and C_2F_3 to form C_3F_6 at different temperatures.

Temperature (K)	C_3F_6
298	-404.86
398	-385.82
498	-366.84
598	-347.93
698	-329.11
798	-310.39
898	-291.76
998	-273.22
1098	-254.76
1198	-236.38
1298	-218.08