**Complete defluorination of 6:2 FTCA in IEX regeneration wastewater: comprehensive comparison of UV/S and UV/PS**

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Table of Contents

[Experimental setup- Figure S.1 2](#_Toc175341126)

[Matrix of regeneration wastes- Text S.1 3](#_Toc175341127)

[Experimental procedure- Text S.2 3](#_Toc175341128)

[UV Fluence Measurement- Text S.3 4](#_Toc175341129)

[SPE purification- Text S.4 5](#_Toc175341130)

[PFAS Measurement- Text S.5 6](#_Toc175341131)

[Ions Measurement- Text S.6 6](#_Toc175341132)

[Quality Assurance/ Quality Control (QA/QC)- Text S.7 7](#_Toc175341133)

[Free energy calculation- Text S.8 7](#_Toc175341134)

[List of associated reactions- Text S.9 8](#_Toc175341135)

[PSO algorithm- Text S.10 14](#_Toc175341136)

[Gibbs free energy landscape- Figure S. 2 15](#_Toc175341137)

[Radical distribution in UV/PS and UV/S treatment of 6:2 FTCA in NaOH containing regeneration waste – Figure S.3-7 17](#_Toc175341138)

[Effect of operational parameter on UV/S defluorination of 6:2 FTCA in NaOH containing regeneration waste – Text S. 11 20](#_Toc175341139)

[Performance of different regeneration wastes under UV/S – Text S. 12 23](#_Toc175341140)

[Chemical scavenging analysis in UV/PS treatment – Figure S.11 27](#_Toc175341141)

[Role of reactive species at different pH – Figure S.12 28](#_Toc175341142)

[Impact of key parameters on distribution of radicals in UV/PS treatment of 6:2 FTCA in Na2SO4 containing regeneration wastes – Figure S.13-16 28](#_Toc175341143)

[Abundance of non-quantified intermediates in UV/PS treatment of 6:2 FTCA in Na2SO4 containing regeneration wastes – Figure S.17 31](#_Toc175341144)

[Gibbs free energy landscape for 6:2 FTCA by · attack – Figure S.18 32](#_Toc175341145)

[Species distribution for S (IV) at different pH – Figure S.19 33](#_Toc175341146)

# **Experimental setup- Figure S.1**

Figure S.1 demonstrates a collimated beam reactor(a) and a flow through reactor (b).

|  |
| --- |
| A picture containing diagram  Description automatically generated  **(a)** |
| Diagram  Description automatically generated  **(b)** |

**Figure S. 1 Schematic diagram of experimental setup (a) collimated beam reactor, (b) flow through reactor (1: feed reservoir, 2: pump, 3: flowmeter and 4: photoreactor).**

# **Matrix of regeneration wastes- Text S.1**

Table S. 1 indicates regenerants with various composition for regeneration of PFAS- saturated resin. Type and concentrations of selected regenerants was selected based on previous studies on regeneration of saturated resins 1-7.

**Table S. 1 composition of regenerants for regeneration of PFAS- saturated IEX resin**

|  |  |  |  |
| --- | --- | --- | --- |
| Regeneration Solution | Concentration (%V/W) | | |
| Level (1) | Level (2) | Level (3) |
| NaCl | 1 | 5.5 | 10 |
| Na2SO4 | 1 | 5.5 | 10 |
| Na2SO3 | 1 | 5.5 | 10 |
| NaHCO3 | 1 | 4.5 | 8 |
| NaOH | 0.5 | 1.5 | 2.5 |
| NH4Cl | 1 | 5.5 | 10 |
| NH4OH | 0.5 | 1.5 | 2.5 |

# **Experimental procedure- Text S.2**

Then, 17 mL of waste was irradiated in a circular petri-dish (diameter: 47 mm) serving as a stirred reactor chamber in the CBR. Samples were collected for analysis at set intervals. To avoid further reaction of residual PS, it was quenched by 0.1 M sodium thiosulfate. The low-pressure lamp emitting light at 254 nm (Light Source Inc. HVA357T5L) was located 29 cm above the waste sample, and the delivered fluence rate was calculated as ~ 0.42 mW.cm-2 using the iodide/iodate actinometry method described by Bolton and Linden (Text S3) 8. In addition to the CBR, a flow through reactor (FTR, Fig S1(b)) with an average fluence rate of ~ 17.2 mW.cm-2 was employed when a relatively high UV fluence was required for degradation. The average fluence rate was quantified using degradation of CBZ (as a model compound) in both CBR and FTR, resulted in creation of a dose-response curve. The average fluence was then determined through back calculation or reduction equivalent fluence (REF) 9. For experiments in the FTR, 1L of prepared waste was irradiated and recirculated with a flow rate of 3L.min-1, and samples were taken at specific time intervals. As described earlier, PS quenching was performed in UV/PS experiments. The external diameter, length, and volume of the FTR were measured as 5.5 cm, 50 cm and 0.3L, respectively, and source of radiation was a 24 W low pressure lamp, emitting UV at 254 nm at the axial center of the reactor.

# **UV Fluence Measurement- Text S.3**

To calculate the fluence applied in the flow-through reactor, degradation of CBZ (as a model compound) employing UV/PS treatment was studied in the flow through reactor. In parallel, CBZ destruction was investigated in the UV- collimated beam reactor. Calculating UV dose in the collimated beam reactor using following procedure, a dose- response curve was conducted for CBZ decomposition. Then, the dose-response curve was applied as a standard curve for back calculation of the UV dose or reduction equivalent fluence (REF) in the flow-through reactor.

To measure photon energy, iodide/iodate actinometry technique was used. In this method, a standard solution, containing 0.6 M KI, 0.1 M KIO3 and 0.01 M Na2B4O7· 10 H2O (borax) at pH 9.25, exposes to UV irradiation which results in generation of triiodide (eq. S1).

|  |  |
| --- | --- |
|  | (eq. S1) |

To calculate UV fluence, absorbance of triiodide was measured spectrophotometrically (eq. S2).

|  |  |
| --- | --- |
|  | (eq. S2) |

Where A352(blank) and A352(sample) are absorbance of the standard solution at 352 nm before and after irradiation, respectively. The constant of 23.373 is obtained by dividing the energy of a mole of photons at 254 nm (4.716 x 105 J Einstein-1) over the product of the quantum yield (0.73) at 254 nm and molar absorption coefficient of triiodide (27600 M-1 cm-1) at 352 nm.

The average fluence delivered to the sample in the collimated beam system, was calculated as following (eq. S3).

|  |  |
| --- | --- |
|  | (eq. S3) |

# **SPE purification- Text S.4**

Weak-ion-exchange SPE cartridges (Waters Oasis Wax, 3mL, 60 mg sorbent) were used with injection of internal standard. First, cartridges were conditioned with 5mL 0.1% NH4OH in MeOH, followed by 5 mL MeOH and 5 mL Milli-Q water. Upon conditioning, 10 mL of well-shaken samples were loaded onto the cartridges with a flow rate of 2 drops.sec-1, and then cartridges were washed with 10 mL 25mM sodium acetate. The cartridges were finally eluted in sequence with 5mL MeOH and 5mL 0.1% NH4OH in MeOH.

# **PFAS Measurement- Text S.5**

Samples were analysed using an Agilent 1200 series HPLC system. 20 of samples was loaded into Waters Xterra MS C18 column (100 2.1 mm, 3.5m particle size; Waters Corporation, Milford, MA), connected to a guard column C18 guard column (30 2.1 mm, 3.5 m particle size) from the same manufacturer. For both column, temperature was set at 50 . Mobile phase consists of 20 mM ammonium acetate (A) and acetonitrile (B) with flow rate of 0.7 mL/min. Elution gradient (A: B) was 50:50 (0 min), 10:90 (0- 5 min), 50:50 (5- 5.5 min) and was held for 2.5 min (5.5- 8 min). An Agilent mass spectrometer (Agilent Technologies, CA, USA) in electrospray negative ionization and multiple reaction monitoring (MRM) modes were employed for mass spectrophotometric analysis. Concentration of target PFAS was quantified using 10-points calibration curve. Table S1 summarizes limit of detection (LOD) and limit of quantification (LOQ) for calibration curve of different PFAS with concentration ranges up to 2 ppm.

**Table S. 2 Studied PFAS with their corresponding calibration curve information.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Name | Chemical structure | m/z | LOD (ppb) | LOQ (ppb) |
| 6:2 FTCA |  | 377 | 4 | 5.2 |
| 6:2 FTUA |  | 357 | 2.32 | 3.81 |
| PFHpA |  | 363 | 0.7 | 0.21 |
| PFHxA |  | 313 | 0.33 | 0.58 |
| PFPeA |  | 263 | 0.35 | 0.8 |
| PFBA |  | 213 | 0.61 | 1.8 |
| PFPrA |  | 163 | 0.20 | 0.48 |
| TFA |  | 113 | 16 | 35.3 |

# **Ions Measurement- Text S.6**

The concentration of persulfate was determined using a spectrophotometric technique described by Liang et al. 10. The sulfite concentration during the reaction was investigated using a Hanna sulfite test kit based on iodometric titration 11. The concentration of inorganic ions in the extracted samples was also measured using an ion chromatograph instrument (Dionex ICS-1100), to ensure their residual concentration is negligible and is not negatively impacting the ionization efficiency and therefore PFAS detection.

# **Quality Assurance/ Quality Control (QA/QC)- Text S.7**

In all experiments, synthetic wastewaters were reproduced and irradiated three times, and associated errors are reported as standard deviation. Instrumental errors for uHPLC/MS including errors arising from different injections of one sample and data processing were calculated to be less than 3.7%. Instrumental errors for the ion selective electrode in fluoride measurement were less than 2.14%, and difference in quantification of fluoride concentration using IC and the ion selective electrode was 5.1%. SPE recovery was assessed through analysis of samples spiked with known concentrations of 6:2 FTCA/ 6:2 FTUA and subsequently comparing the detected analyte concentrations in the extracted samples to the known spiked concentrations. For all wastewaters with different compositions, SPE recovery was determined to be above 95.2%.

# **Free energy calculation- Text S.8**

The reason to utilize the PBE was its superiority and reliability in dealing with processes involving electron transfer. To enhance the self-consistent field calculations 12, 13, thermal smearing 14 and double numerical basis including d-polarization function level of theory were used 15. The convergence tolerances were set at energy: 2.0×10-5 kcal/mol, force: 10-3 kcal/mol/Å, max iterations: 104, displacement: 10-5 Å. The Hirano’s formulation 16 was used to extract thermodynamic properties inclusive of Zero-point vibrational energy (ZPVE), particularly the Gibbs free energy. To get an understanding of how electron transfer may occur, the LUMO (lowest unoccupied molecular orbital) profiles, particularly for 6:2 FCTA and 6:2 FTUA were determined.

# **List of associated reactions- Text S.9**

Table S2 and S3 reports the reactions and their corresponding rate constants may occur in UV/PS and UV/S degradations, respectively.

**Table S. 3 Reactions in UV/PS treatment of FTCA within different regeneration wastes 17-20**

|  |  |
| --- | --- |
| Reactions | K (M-1 s-1) |
|  | = 0.50 mol/Einstein;  = 22.07 M-1 cm-1 |
|  | K[=17800 s-1 |
| + → - | 1010 |
|  | 1.4 107 |
|  | > 2 109 |
|  | 1.3 1010 |
|  | 9.4 107 |
|  | 1.4 108 |
|  | 5.5 10-6 s-1 |
|  | 4.2\* 109 |
|  | 5 108 |
|  | 5.7104 |
|  | 6.8 109 |
|  | 3.8109 |
|  | 2.7107 |
|  | 1.21010 |
|  | 4 108 |
|  | 5.5 \*109 |
|  | 5.21010 |
|  | 3.3 102 s-1 |
|  | 8105 s-1 |
|  | 5 1010 |
|  | 3.9107 |
|  | 7109 |
|  | 6.6109 |
|  | 1.11010 |
|  | 2.7107 |
|  | 1.1 105 s-1 |
|  | 9 1010 |
|  | 5107 |
|  | 2 1010 |
|  | 9.7 107 |
|  | 8.3105 |
|  | 1.8 105 |
|  | 0.095 |
|  | = 8.30 10-4 s-1 |
|  | 3.74 105 |
|  | 8.2 109 |
|  | 9.92 109 |
|  | 1.2 107 |
|  | 3.5 109 |
|  | 1.2 107 |
|  | 1.0 1010 |
|  | 1.0 106 |
|  | 2.1 108 |
|  | 2.2 108 |
|  | 8.96 109 |
|  | 4.4 104 (fitted) |
|  | 2.5 104 (fitted) |
|  | 3 105 |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
| + |  |
|  | 2.5 108 |
|  | = 1.30 103 s-1 |
|  | 2.1 1010 |
|  | 1.0 104 |
|  | 8.0 109 |
|  | 5.3 104 s-1 |
|  | 8.8 107 |
|  | 6.41 109 |
|  | 2.1 109 |
| . | 1.4 105 |
|  | 3.0 109 |
|  | = 1.30 103 s-1 |
|  | 1.0 102 |
|  | 5.0 109 |
|  | 1.0 108 |
|  | 2.0 109 |
|  | 1.0 109 |
|  | = 15 s-1 |
|  | 2.0 109 |
|  | 8.8 109 |
|  | 3.0 109 |
|  | 8.2 109 |
|  | 1.0 109 |
|  | 4.0 109 |
|  | 2.79 109 |
|  | 8.23 109 |
|  | 7.8 105 |
|  | 9.4 108 |
| byproducts | 5.04 10-6 |
|  | pKa= 7.6 |
|  | 4.3 105 |
|  | pKa = 10.3 |
|  | Ka= 1.8 10-5 |
|  |  |
|  | 9.0107 |
| **6:2 FTCA decomposition in hydroxide containing regeneration wastewater** | |
|  | 8.8×108 (fitted) |
|  | 1.7×1010 (fitted) |
|  | 1.05×1010 (fitted) |
|  | 3.12×109 (fitted) |
|  | 7.56×108 (fitted) |
| **6:2 FTCA decomposition in remaining regeneration wastewaters** | |
|  | 1.3×1011 (fitted) |

**Table S. 4 Reactions in UV/S treatment 18, 19, 21, 22**

|  |  |
| --- | --- |
| Reactions | K (M-1 s-1) |
|  | mol/Einstein, |
|  | 8.3105 |
|  | 9.7 107 |
| SO4•− + HO• → HSO5- | 1010 |
|  | 1.5 109 |
|  | (5.5-9.0) 106 |
|  | 1.4 107 |
|  | > 2 109 |
|  | 3.1 108 |
|  | 2 105 |
|  | 2 107 |
|  | 3 1010 |
|  | 1.3 1010 |
|  | 9.4 107 |
|  | 1.4 108 |
|  | 5.5 10-6 s-1 |
|  | 4.2 109 |
|  | 5 108 |
|  | 5.7104 |
|  | 6.8 109 |
|  | 1.8 1010 |
|  | 103s-1 |
|  | < 1.5106 |
|  | 2.8 1010 |
|  | 3.4 1010 |
| 2 | 6109 |
|  | 3.5109 |
|  | 2.5107 |
|  | 3.8109 |
|  | 2.7107 |
|  | 1.21010 |
|  | 4 108 |
|  | 5.5 109 |
|  | 5.21010 |
|  | 3.3 102 s-1 |
|  | 8105 s-1 |
|  | 5 1010 |
|  | 3.9107 |
|  | 7109 |
|  | 6.6109 |
|  | 1.11010 |
|  | 2.7107 |
|  | 1.1 105 s-1 |
|  | 9 1010 |
|  | 1.31010 |
|  | 5107 |
|  | 2 1010 |
|  | 9.7 107 |
| **6:2 FTCA decomposition in hydroxide containing regeneration wastewaters** | |
|  | 8.8×108 (fitted) |
|  | 1.7×1010 (fitted) |
|  | 1.05×1010 (fitted) |
|  | 3.12×109 (fitted) |
|  | 7.56×108 (fitted) |
| + +byproducts | 108 |
| + +byproducts | 108 |
| + +byproducts | 108 |
| + +byproducts | 108 |

# **PSO algorithm- Text S.10**

The conventional trial-and-error approach in calculating the unknown rate constants is not reliable and time-consuming. Thus, we used a heuristic optimization algorithm, here particle swarms (PSO), to determine the optimal value of unknown rate constants. In PSO, a swarm of particles (set of guesses for rate constants) moves around a search space, seeking to find the optimal solution (minimized error between calculated and experimentally measured concentration). The position of each particle (values of rate constant in each guess set) in the search space represents a potential solution. In PSO the values of each rate constant (particle’s position and velocity) is updated over a number of iterations (known as generation) respectively as and .

Here, is the velocity of particle, is the inertia weight (a hyperparameter that controls the particle's tendency to maintain its velocity), and are the acceleration coefficients (hyperparameters that control the influence of the particle's personal best position and the swarm's global best position on its velocity), is a random number generator, t is the personal best position of particle, is the current position of particle, and is the global best position of the swarm.

We compute the error between calculated and experimentally measured concentration using the SD (standard deviation) formula given as follow.

|  |  |
| --- | --- |
|  | (eq. S4) |

Where n is the number of data points achieved under the same operational conditions. and are experimental and modeled concentration of the target PFAS, respectively. Once the SDs are computed for all particles in each iteration, the minimum value in SD is identified and assigned as . The values of over interactions are compared, and the smallest is assigned as . We designed the initial set of initial guesses for unknown rate constants to be generated randomly within the physically relevant domain as inspired by an analogy with similar reactions in the literature. The reactions conclude a sophisticated, non-stiff and highly coupled set of ODEs (ordinary differential equation) and therefore, we utilized MATLAB *ode15s* function capability in numerically solving the ODEs (ordinary differential equation) arising from the reactions.

# **Gibbs free energy landscape- Figure S. 2**

Fig. S. 2 indicates the Gibbs free energy landscape for proposed pathways of 6:2 FTUA decomposition by attack.

Shape

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Description automatically generatedA diagram of a chemical formula

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**Figure S. 2 Gibbs free energy landscape for 6:2 FTCA decomposition by attack under alkaline condition**

# **Radical distribution in UV/PS and UV/S treatment of 6:2 FTCA in NaOH containing regeneration waste – Figure S.3-7**

**A graph of a number of objects

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**Figure S. 3 Distribution of .OH in UV/PS treatment of 6:2 FTCA in 0.5% NaOH containing regeneration waste**

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**Figure S. 4 Distribution of in UV/PS treatment of 6:2 FTCA in 0.5% NaOH containing regeneration waste**

A graph of a function

Description automatically generated

**Figure S. 5 Distribution of .OH in UV/S treatment of 6:2 FTCA in 0.5% NaOH containing regeneration waste**

A graph of a function

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**Figure S. 6 Distribution of in UV/S treatment of 6:2 FTCA in 0.5% NaOH containing regeneration waste**

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**Figure S. 7 Distribution of in UV/S treatment of 6:2 FTCA in 0.5% NaOH containing regeneration waste**

# **Effect of operational parameter on UV/S defluorination of 6:2 FTCA in NaOH containing regeneration waste – Text S. 11**

**Concentration of regenerant (CNaOH) –** Application of varying concentrations of NaOH for the regeneration of saturated resins, necessitates evaluation of NaOH concentration on efficiency of degradation process. Compared to the control experiment (without NaOH), remarkable defluorination was observed in the NaOH containing regeneration wastes. The lowest NaOH concentration (0.5% W/V) resulted in highest (complete) defluorination, where increasing concentration to 2.5% W/V, slightly reduces defluorination to 82%. The optimum concentration of 0.5% W/V for NaOH is explained by generation of in presence of , facilitating decomposition of 6:2 FTUA and release of fluoride. Excess concentration of leads to more production of and thereby greater concentration of PFCAs. The higher generation of , on the other hand, consumes rapidly, and consequently, reduces defluorination efficiency. Therefore, in NaOH containing regeneration wastes, interplay of and is a key factor and even may exert a substantial adverse implication on decomposition of PFAS with no reactivity toward such as PFOA and PFOS.

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**Figure S. 8 Effect of regenerant concentration on defluorination efficiency (DO= 8ppm, Csulfite= 30 mM)**

**Sulfite dose () –** effect of sulfite concentration was investigated on defluorination from 7.5 mM to 30 mM. Sulfite is essential for generation of both key agent of and . As depicted, defluorination increases from 69.3% to 100% when sulfite concentration enhances from 7.5 mM to 15 mM. Variation of sulfite concentration from 15 mM to 30 mM, on the other hand, did not affect the defluorination significantly, which is probably attributed to scavenge of . Compatible with defluorination results, intermediates measurement indicated same intermediates with equal concentrations at sulfite concentrations ranging from 15 mM to 30 mM, suggesting 15 mM sulfite as the optimum concentration for complete defluorination in NaOH containing regeneration wastes.

A graph of different colored lines

Description automatically generated

**Figure S. 9 Effect of sulfite concentration on defluorination efficiency (DO= 8ppm, CNaOH= %0.5 W/V)**

**Dissolved Oxygen –** effect of dissolved oxygen was investigated through sparging nitrogen into the solution. While O2 is known to scavenge (= 1.8× 1010) and can negatively affect the -based degradation, decrease in O2 to 0.4 ppm causes negligible defluorination (10.3%). The positive role of O2 is due to its impact on generation (eq 3, 20 and 21), the main initiating agent in decomposition of 6:2 FTUA. Additionally, as suggested by pathway (Fig. 1), degradation of 6:2 FTUA happens by and O2 attack. Therefore, UV/S defluorination of 6:2 FTUA not only is influenced negatively by O2, but also benefit from it, suggesting potential application of UV/S treatment of 6:2 FTCA in open-air systems.

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Description automatically generated

**Figure S. 10 Effect of sulfite concentration on defluorination efficiency (Csulfite= 30 mM, CNaOH= %0.5 W/V)**

# **Performance of different regeneration wastes under UV/S – Text S. 12**

Efficiency of UV/S technique for 6:2 FTCA degradation in the remaining regeneration wastes (i.e., NaCl, NH4Cl, Na2SO4, Na2SO3 andNaHCO3) was investigated. The results (**Figure S. 11** b) indicated negligible to low degradation of 6:2 FTCA within the fluence of 248 J.cm-2 for most regeneration wastes including NaCl (20.8%), NH4Cl (0%), Na2SO4 (18.1%) and NaHCO3 (6%). Furthermore, no to negligible defluorination ( 4.62%) was obtained for the studied regeneration wastes, indicating inefficient performance of UV/S. These observations are consistent with literature 23 on UV/S treatment of aqueous film forming foam (AFFF), reporting inefficiency of UV/S at treating shorter chain PFAS such as PFSAs and FTSAs (total defluorination of 53% 23).

|  |
| --- |
| **(a)**  A graph of a line with dots  Description automatically generated with medium confidence |
| A picture containing screenshot, text, line, plot  Description automatically generated  **(b)** |
| **Figure S. 11 6:2 FTCA degradation in different synthetic regeneration wastewaters (CPS/S= 15mM and C6:2FTCA= 10 ppm) using (a) UV/PS and (b) UV/S treatments** |

The presence of CH2 moieties in the molecular structure of 6:2 FTCA could explain this observation, which makes the C-F bond on the neighboring carbons distinctively recalcitrant, thereby suppresses the ability of in decomposing fluorotelomers. Considering 31.5% decomposition in the control experiment (without regenerant), it can be realized that bimolecular scavenging reactions also played a role in observed insignificant UV/S decomposition as suggested by eqs. S5-7 22. In addition to chemical structure and reactivity of 6:2 FTCA toward , and impact of ions on scavenging , contribution of regenerants to fraction of protonated/deprotonated form of sulfite is significant. For instance, as discussed in previous chapters, acidic condition of regeneration waste as a result of presence of 10% NH4Cl regenerants is not favorable for existence and action of (Fig. S19) 24, leading to lower performance of NH4Cl compared to other chloride containing regeneration wastes such as NaCl.

|  |  |  |
| --- | --- | --- |
|  | @pH= 7 | (eq. S5) |
|  |  | (eq. S6) |
|  |  | (eq. S7) |

Among the aforementioned five regenerants, highest efficiency (51.1% degradation and 38.3% defluorination) was achieved from photolysis of 10% Na2SO3 containing regeneration wastes within fluence of 248 J.cm-2, that is orders of magnitude less efficient compared to results of UV/PS treatment (**Figure S. 11** a). At excess concentration of sulfite, higher amount of and consume (eq. S12, 13). Greater generation of produces greater amount of that consequently causes scavenge of (eqs. S8-10) 25. Additionally, undergoes self-scavenging at high concentrations (eq. S11). Therefore, the overall mild performance of sulfite containing regeneration wastes can be attributed to two key factors: the inherent resistance of the 6:2 FTCA structure (and its potential intermediates with similar structure) towards and the scavenging of . Hence, it can be concluded the direct utilization of UV/S for decomposing 6:2 FTCA within regeneration wastes (comprising various salts excluding hydroxide salts) is neither efficient nor economically viable.

|  |  |  |
| --- | --- | --- |
|  |  | (eq. S8) |
| + |  | (eq. S9) |
| + |  | (eq. S10) |
|  |  | (eq. S11) |
|  |  | (eq. S12) |
|  |  | (eq. S13) |

# **Chemical scavenging analysis in UV/PS treatment – Figure S.11**

As depicted in Figure S. 12, · is responsible element for degradation of 6:2 FTCA in different matrices.

|  |
| --- |
| A graph of a number of green bars  Description automatically generated with medium confidence  **(a)** |
| A graph of different sizes of numbers  Description automatically generated with medium confidence  **(b)** |

**Figure S. 12 Chemical scavenging analysis for (a) Na2SO4 containing regeneration wastes (within fluence of 125 mJ/cm2), (b) Chloride containing regenerants (within fluence of 31000 mJ/cm2)**

# **Role of reactive species at different pH – Figure S.12**

According to Figure S. 13, at pH4, · is the dominant species in initiation of 6:2 FTCA decomposition.

Chart, bar chart

Description automatically generated

**Figure S. 13 contribution of · and** **On degradation at different pH**

# **Impact of key parameters on distribution of radicals in UV/PS treatment of 6:2 FTCA in Na2SO4 containing regeneration wastes – Figure S.13-16**

Figure S 13-16 shows effect of influencing parameters on distribution of radicals in UV/PS treatment of 6:2 FTCA in 10% Na2SO4 containing regeneration waste.

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**Figure S. 14 effect of pH on · distribution in UV/PS treatment of 6:2 FTCA in10% Na2SO4 containing regeneration wastes**

A graph of ph and ph values

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**Figure S. 15 effect of pH on distribution in UV/PS treatment of 6:2 FTCA in10% Na2SO4 containing regeneration wastes**

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**Figure S. 16 effect of persulfate dose on · distribution in UV/PS treatment of 6:2 FTCA in10% Na2SO4 containing regeneration wastes**

A graph of different colored lines

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**Figure S. 17 effect of initial concentration of 6:2 FTCA on · distribution in UV/PS treatment of 6:2 FTCA in10% Na2SO4 containing regeneration wastes**

# **Abundance of non-quantified intermediates in UV/PS treatment of 6:2 FTCA in Na2SO4 containing regeneration wastes – Figure S.17**

A graph of a number of people

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**Figure S. 18 Peak area for non-quantified intermediates in UV/PS treatment of 6:2 FTCA in 10% Na2SO4 containing regeneration waste**

# **Gibbs free energy landscape for 6:2 FTCA by *·* attack – Figure S.18**

Diagram

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Diagram

Description automatically generated with medium confidence

Diagram

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**Figure S. 19 Gibbs free energy landscape for 6:2 FTCA degradation by · attack**

# **Species distribution for S (IV) at different pH – Figure S.19**



**Figure S. 20 Species distribution of S(IV) at pH range from 0.00 to 14.00.**

**References**

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