Electronic supplementary information (ESI)

Leachability of Per- and Poly-Fluoroalkyl Substances from Contaminated Concrete

Prashant Srivastava, [*a] Grant Douglas, [b] Greg B. Davis, [b] Rai Kookana, [a] Canh Tien Trinh Nguyen, [a] Mike Williams, [a] Karl Bowles, [cd] and Jason K. Kirby [a]

[a] Commonwealth Scientific and Industrial Research Organization, Environment Business Unit, Industry Environments Program, Waite Campus, Urrbrae, SA 5064, Australia

[b] Commonwealth Scientific and Industrial Research Organization, Environment Business Unit, Industry Environments Program, 7 Conlon St, Waterford, WA 6152, Australia

[c] Jacobs, L7/177 Pacific Hwy, Jacobs, North Sydney, 2060, Australia

[d] Queensland Alliance for Environmental Health Sciences (QAEHS), The University of Queensland, Cornwall Street, Woolloongabba, QLD, 4102, Australia

* Corresponding author

Email: Prashant.Srivastava@csiro.au

SI 1. Calculations of total PFAS in concrete monoliths (µg/kg), the proportion of PFAS leached at sampling points (%), cumulative mass (µg) and proportion leached (%), and rate of PFAS leached (%/d).

Total PFAS concentrations in the concrete monoliths were determined at the completion of the test as follows:

$$CT_{PFAS} = \frac{ML_C + M_R}{W} \quad \text{Eq (i)}$$

where:

$CT_{PFAS} = Total\ concentration\ (\mu g/kg)\ of\ PFAS\ in\ monolith$

$ML_C = Cumulative\ mass\ (\mu g)\ of\ PFAS\ leached\ from\ monolith$

$M_R = Residual\ mass\ (\mu g)\ of\ PFAS\ in\ monolith$

$W = Weight\ (kg)\ of\ monolith$

The proportion of PFAS leached at a given sampling time point (t) was calculated as a percentage of the total PFAS concentration in the monoliths as follows:

$$PL_t = \frac{ML_t}{MT_{PFAS}} \times 100 \quad \text{Eq (ii)}$$

where:

$PL_t = Proportion\ (\%)\ of\ PFAS\ leached\ from\ monolith\ at\ a\ given\ sampling\ time\ point, t$

$ML_t = Mass\ (\mu g)\ of\ PFAS\ leached\ from\ monolith\ at\ the\ given\ sampling\ time\ point, t$

$MT_{PFAS} = Total\ mass\ (\mu g)\ of\ PFAS\ in\ monolith$

The cumulative proportion of PFAS leached at each sampling time point in the test was calculated as a percentage of the total PFAS concentration in the monoliths as follows:

$$PL_{C,t} = \frac{ML_{C,t}}{MT_{PFAS}} \times 100 \quad \text{Eq (iii)}$$

where:

$PL_{C,t} = Cumulative\ proportion\ (\%)\ of\ PFAS\ leached\ from\ monolith\ at\ a\ given\ sampling\ time\ point, t$

$ML_{C,t} = Cumulative\ mass\ (\mu g)\ of\ PFAS\ leached\ from\ monolith\ at\ the\ given\ sampling\ time\ point, t$

$MT_{PFAS} = Total\ mass\ (\mu g)\ of\ PFAS\ in\ monolith$

The cumulative mass (µg) of PFAS leached from monolith at the given sampling time point was calculated by summation of the mass of PFAS leached at each sampling time point up until the given sampling time point. The total mass of PFAS in the monolith was calculated by adding the

cumulative mass (µg) of PFAS leached from the monolith and the residual mass (µg) of PFAS in the monolith after leaching.

The rate of leachability for PFOS, PFOA, PFHxS, and PFHxA from contaminated concrete monoliths was calculated [Eq (iv)] across different time points to understand the leaching mechanisms as follows:

$$Rate\ of PFAS\ leachability\ (\%/d) = \frac{PFAS\ leached\ (\%)\ at\ a\ given\ sampling\ time\ point}{Sampling\ interval\ (d)} \quad \text{Eq (iv)}$$

The rate was calculated for each concentration level (low, intermediate, and high) of the monoliths at different sampling time points. Two mean rates were determined: (a) Mean M-SI, representing the average leachability rate across all monoliths at a given sampling interval, irrespective of concentration level; and (b) Mean M-C, representing the average leachability rate for each concentration level, irrespective of the sampling interval. Mean M-SI was calculated for each sampling interval (0.08, 0.92, 1, 5, 7, 14, and 28 d), with one sample for most intervals except two samples for 7 d and three samples for 14 d. Mean M-C was calculated by averaging the leachability rates of monoliths within each concentration level across all sampling intervals.

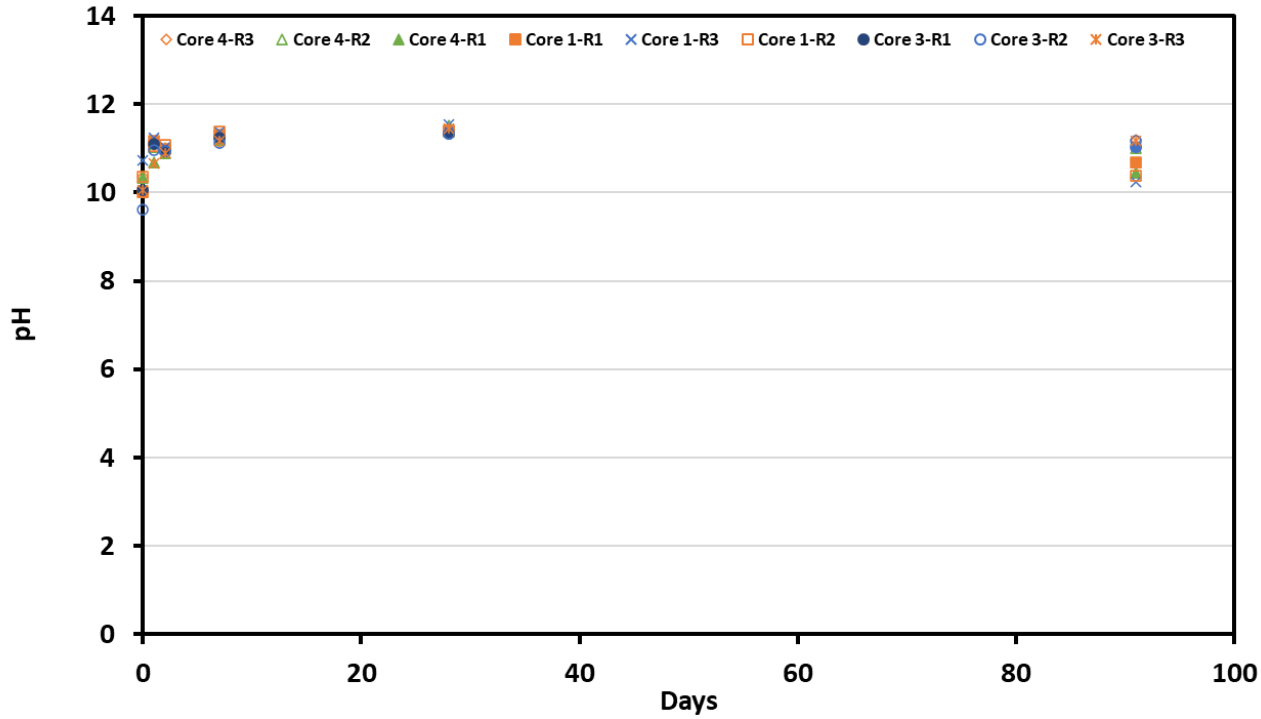
SI 2. Limit of quantitation (LOQ) in concrete solids and leachate.

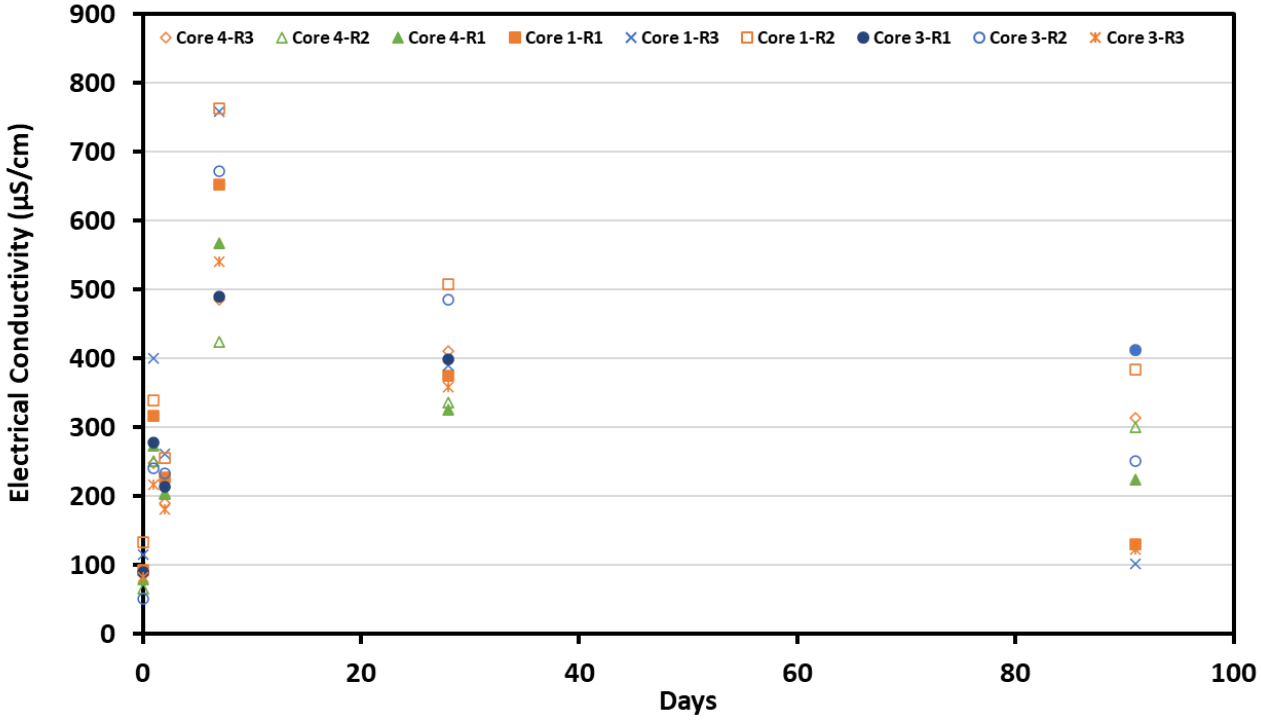
µg/kg	1	1	1	1
ng/L	3	3	3	3

SI 3. Moles of 4 *M* HNO_3 required to achieve pH in powdered concrete suspensions after 6 d.

11	0.050
9	0.770
7	1.831

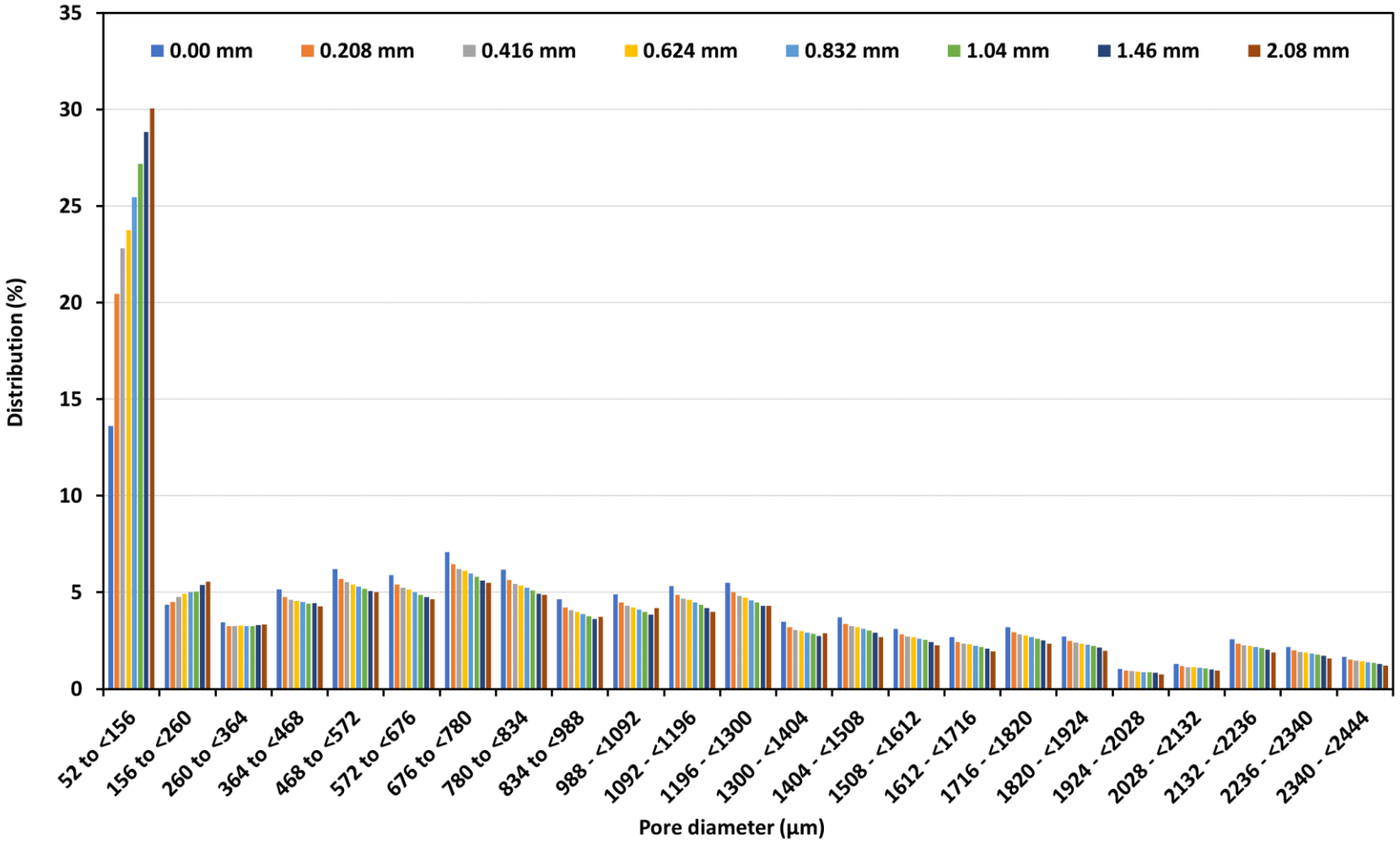
SI 4. Change in pH and electrical conductivity over time in LEAF method 1315 study of contaminated concrete monoliths.



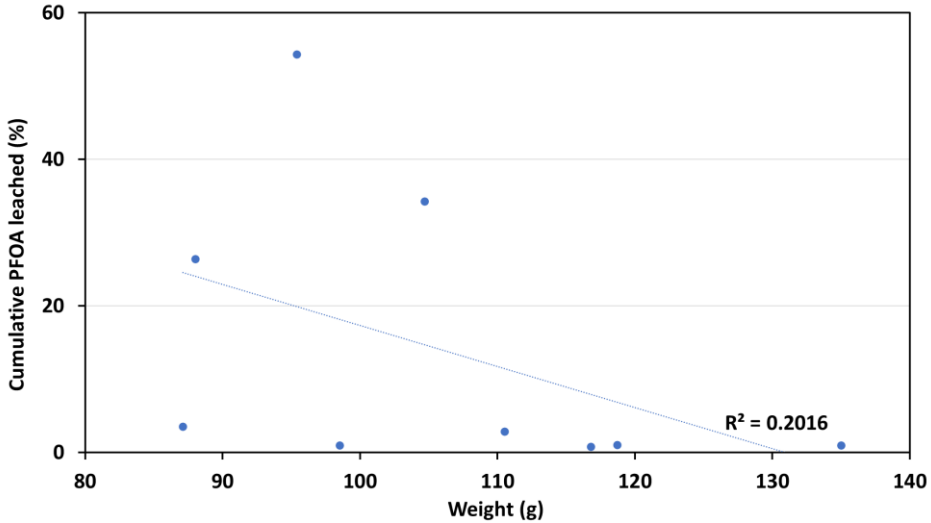


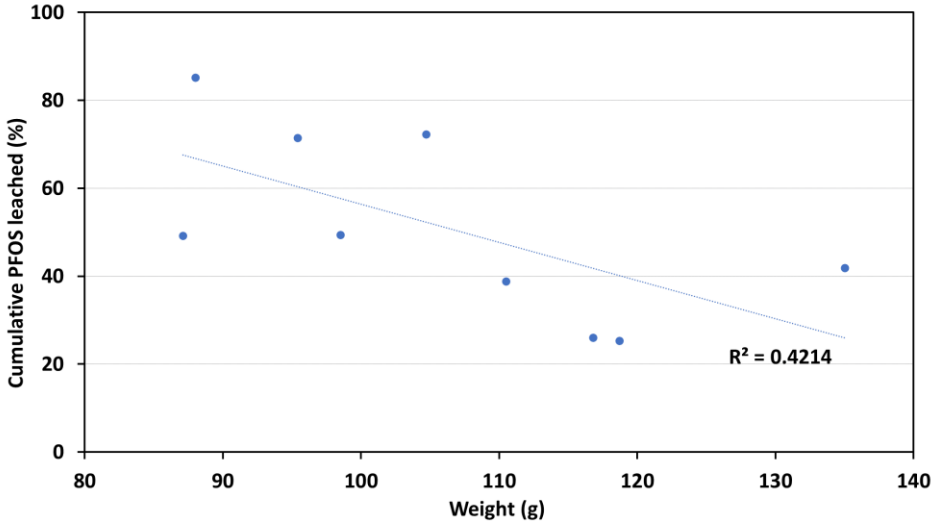
SI 5. Pore diameter distribution (%) within a concrete monolith sample at different shrink-wrap applied in 3D with "0.00 – 2.08 mm stretch" clinging to the outer boundary of the concrete monolith.

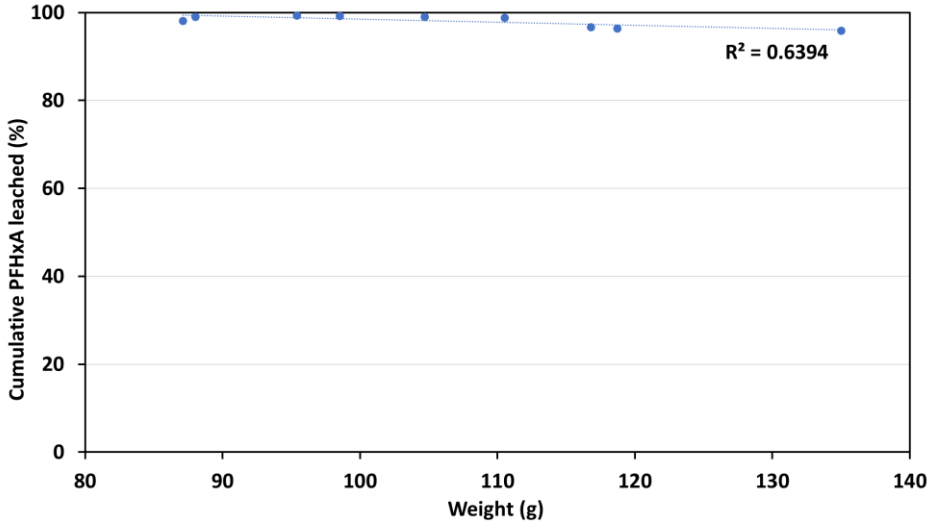
To determine the external boundary, external surface area and volume of the concrete half-puck, a "Region of Interest (ROI) shrink-wrap" plug-in algorithm was applied in 3 dimensions (3D), which conformed the ROI boundaries to the outer surface of the sample (i.e. the conforming to the contours of the samples where water could potentially fill) and "stretching" over "open pores" (i.e. pores connecting to the sample surface) with a maximum opening (diameter) of 2.08 mm (as pores in concrete wouldn't be expected to be larger than 2 mm).

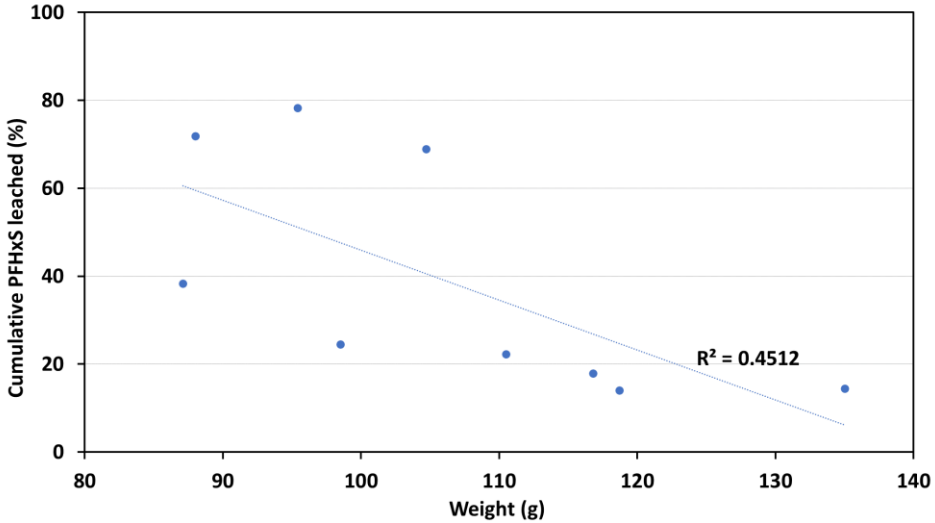


SI 6. Relationships between cumulative % PFAS leached and concrete monolith mass.

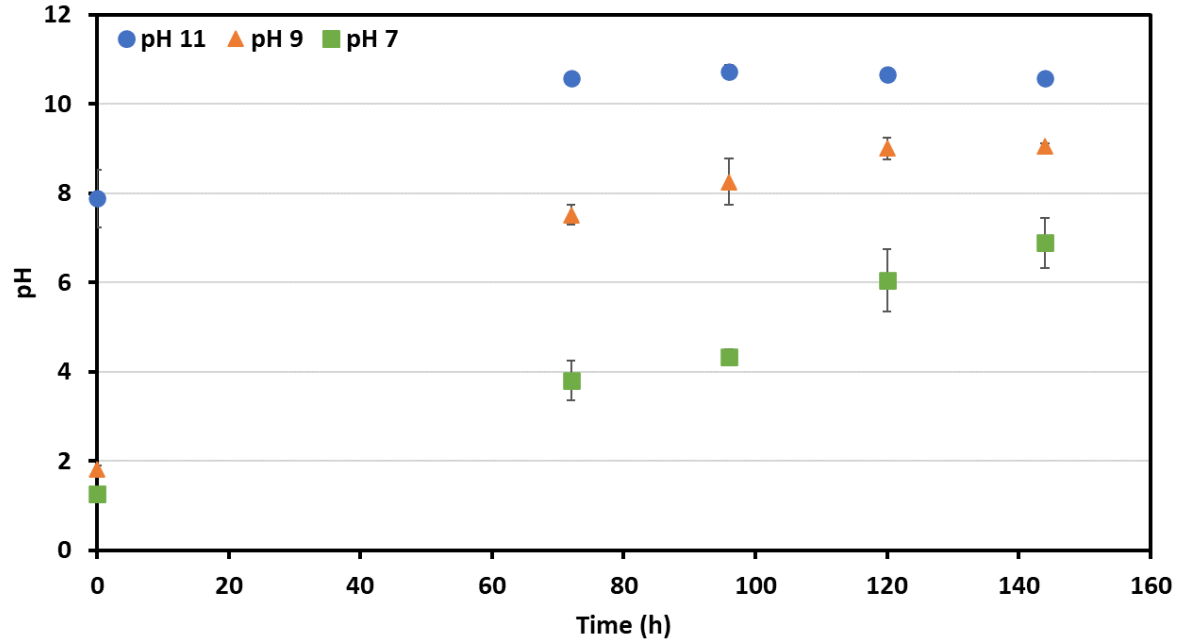


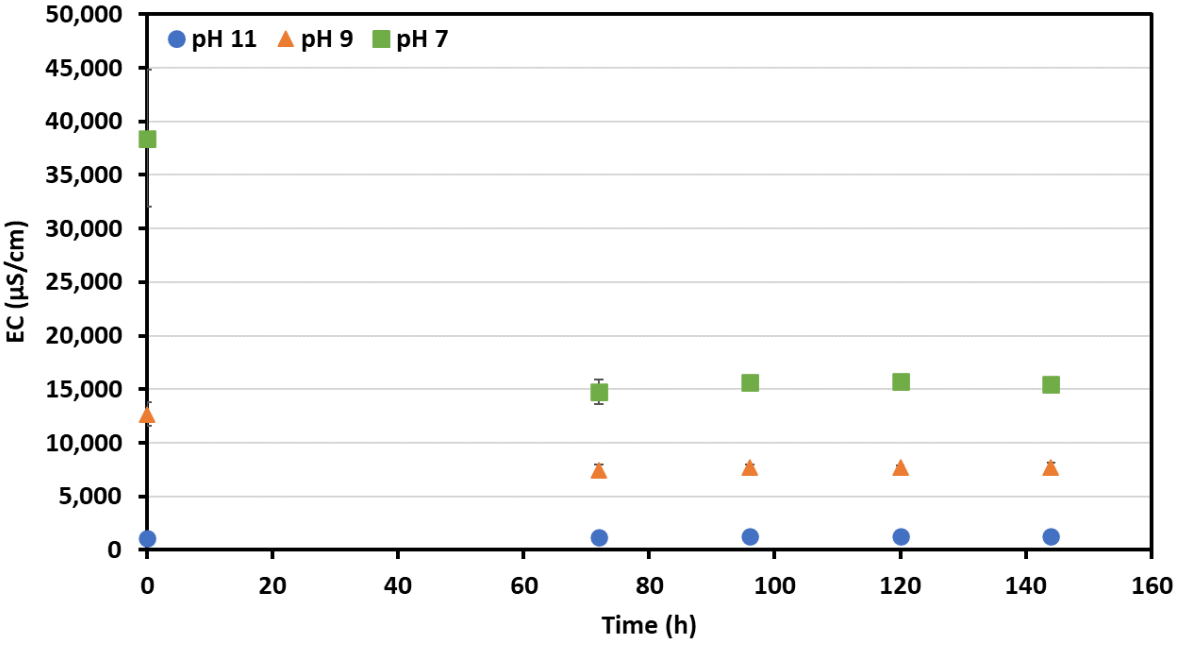






SI 7. Change in pH and electrical conductivity over time in LEAF method 1313 study of contaminated powdered concrete.





SI 8. Depth profile for PFHxA concentration (µg/kg) for cores 1, Core 3 and Core 4.