Mathematical Study on Prey-Predator Dynamics Under Effect of Water Contamination

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Abstract:A significant class of water pollutants emerging as a threat to human and aquaticpopulations is Per-and-polyfluoroalkyl substances (PFAS). The primary concern linked to PFAS is that they exhibit bioaccumulation potential as their perfluorocarbon moieties do not break down or do so very slowly under natural conditions, which is why PFAS has often been termed "forever chemicals." These chemicals are disposed off in aquatic bodies via improper disposal methods, and because PFAS are persistent, they accumulate or concentrate in the water environment. Subsequently, these chemicals hamper the aquatic population and further enter the human food chain via direct consumption of affected aquatic species and drinking water. In this study, a mathematical model has been developed to understand the alarming consequences of PFAS on human and aquatic populations and the various challenges being faced due to inadequate treatment and management of these chemicals. The model has been analyzed for stability at the equilibrium points. Numerical simulations have also been carried out to support the analytical findings. The analysis demonstrates that rising PFAS contamination is extremely hazardous to both aquatic and human populations and immediate control methods need to be devised to restrain their increasing levels in water.

Keywords: Human population, Aquatic population, per and poly-fluoroalkyl substance,Mathematical Modelling, Stability

1 Introduction

PFAS (per- and polyfluoroalkyl substances) are a group of man-made chemicals that have been used in a variety of industrial and consumer products for decades[1]. PFAS exhibits bioaccumulation, which increases with chain length. They are regarded as highly fluorinated surfactants that have been used in the production of electronics, fluoropolymers, clothing, protective coatings for fabrics and carpets, and food packaging, among other industrial uses and manufactured goods [2].These perfluorocarbon moieties typically do not break down or do so very slowly under natural conditions, which is why PFAS are often referred to as "forever chemicals." [3] Fish is known to be an essential source of dietary PFAS, according to studies done across the globe. One noteworthy cause for the increase in the level of PFAS is the quantity of fish and shellfish that are consumed, although this varies with the type of fish or shellfish [4]. PFAS have been found in marine mammals such as polar bears, dolphins, seals, killer whales, and beluga whales [5]. The study showed higher levels of extractable organic fluorine in marine mammals compared to other marine animals and terrestrial animals [6]. One of the most significant food sources of PFAS for humans is seafood, especially when caught in hotspot seas with substantially higher PFAS concentrations than the background [7]. Certain PFAS chemicals adversely affect human health by altering thyroid and kidney function, suppressing the immune system, and hurting development and reproduction [8-10] There are several shortcomings when it comes to accessing the information that is required as far as human health risks are concerned, especially for many PFAS with a wide range of structures and chemical properties [11-13]In-utero openness to existing environmental contaminants such as PFAS is connected with adverse health outcomes during pregnancy, birth outcomes, and later life [14-16]. Specifically, this PFAS has been considered the main reason for the increase in the incidences of gestational diabetes, childhood obesity, preeclampsia, and foetal growth restriction [17]. Due to their environmental durability and toxicity, potential for bioaccumulation, and potential for detrimental health effects, PFASs have recently attracted more and more attention on a global scale [18].

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Mathematical modeling has proven a useful tool in the study of many biological phenomena. The scope of developing thismathematical model is to analyze the effect of PFAS on aquatic and human populations [19]. In this study, we develop a mathematical model to predict the harmful effect of PFAS on aquatic ecosystems and subsequently human population. The existence, uniqueness, and boundness of the system solution are investigated [20].The local stability of the system at equilibrium points is discussed, and the analytical results obtained in the proposed model are justified using numerical simulation.

2Mathematical Modelling

The study focuses on analyzing the population dynamics of a predator-prey system in an aquatic environment, taking into account the impact of elevated levels of PFAS.[21] This model describes the interaction between the concentration of PFAS in aquatic bodies (P), the density of the aquatic population (W), and the density of the human population (H). The model makes it possible to identify the risk to human health from PFAS. In addition to these requirements, the model's development detects dangerous levels of PFAS.[22] The model that has been developed consists of a set of nonlinear differential equations that incorporate the notations that have been previously mentioned. These equations describe the dynamics of a system involving a predator (human population) and prey (aquatic population) relationship in an aquatic environment, with consideration given to the effects of increased levels of PFAS.[23]

$$\frac{dP}{dt} = E - cPW - aPH \tag{1}$$

$$\frac{dW}{dt} = qW(1 - cP) - bW - rWH \tag{2}$$

$$\frac{dH}{dt} = grWH - MaPH - hH \tag{3}$$

Where the initial condition is given by:

$P(0) > 0, W(0) > 0, H(0) > 0$

The following definitions apply to the system parameters:

The first equation describes the rate of change of P with time, which is dependent on the external input of PFAS into the aquatic body (E), the uptake of PFAS by the aquatic population (cW), and the uptake of PFAS by the human population (PH). The uptake rate of PFAS by the aquatic population (c) and human population (a) is assumed to be proportional to the concentrations of PFAS in the water and the human body, respectively.[24]

The second equation describes the rate of change of W with time, which is dependent on the growth of the aquatic population (qW), the predation of the aquatic population by the human population (cPW), and the natural death rate of the aquatic population (bW). Additionally, the growth of the aquatic population is also affected by the presence of PFAS in the water (rWH), which reduces the reproductive rate of the aquatic population.[25]

The third equation describes the rate of change of H with time, which is dependent on the growth of the human population due to consumption of the aquatic population $(grWH)$, the mortality of the human population due to PFAS exposure $(MaPH)$, and the natural death rate of the human population (hH). Additionally, the growth of the human population is also affected by the presence of PFAS in the water (rWH), which reduces the carrying capacity of the aquatic ecosystem.

All the parameters E, c, a, q, b, r, g and $m$are regarded as constant positive variables.

We will perform the mathematical analysis of the model$(1) - (3)$ provided by equations in the parts that follow:

3 Boundedness and dynamical behavior of the model

Boundedness of solutions***:*** To ensure the model's biological validity, we will demonstrate that the system's solutions are bounded. Because model $(1)-(3)$ depicts the human and aquatic population, it is critical that it is statistically significant and that the state variables are nonnegative at any given time t > 0.We therefore ought to demonstrate that the solutions of this model are bounded.

Lemma 1*:* All solutions of the model given by equations shall lie in the region $(1)-(3)$ shall lie in region *Fr* where: $Fr = \{(P, W, H) \in R_+^3 : 0 \leq P + W + H \leq \delta_1\}$ for all $t \to \infty$ with the positive initial value $P(0), W(0), H(0)$ where $\delta_1 = \frac{E}{\beta_1}$, where, $\beta_1 = \min(h, g(b-q), \alpha_1)$ &$\alpha_1 = \min(c, a)$

Proof: Consider the following function $\delta_1$given by:

$$\delta_1 = \mathrm{P} + \mathrm{W} + \mathrm{H}$$

$$\frac{d\delta_1}{dt} = \frac{dP}{dt} + \frac{dW}{dt} + \frac{dH}{dt}$$

From equation $(1)-(3)$ and taking $\alpha_1 = \min(c, a)$ we obtain,

$$\frac{d\delta_1}{dt} \leq E - hH - (gb - gq)W - \alpha_1 P$$

$$\beta_1 = \min(h, gb - gq, \alpha_1)$$

$$\frac{d\delta_1}{dt} \leq E - \beta_1(H + W + H)$$

$$\frac{d\delta_1}{dt} \leq E - \beta_1 \delta_1$$

Then, using the standard comparison theorem, we arrive at:

$$\lim_{t \to \infty} \sup(\delta_1 t) \leq \frac{E}{\beta_1} = \delta_{1u}$$

Hence the lemma is proved

Positivity of Solutions

Since the model given by equations$(1)-(3)$ studies the dynamical behavior of aquatic and human population under the effect of increasing PFAS pollutant, it becomes imperative to prove that the solution exhibit positivity at all times. The following lemma demonstrates the positivity of explanation since positivity implies that solutions endure.

Lemma: The solution of the model given by equation$(1)-(3)$, $\big(P(t), W(t), H(t)\big)$,with initial condition, $P(0) > 0, W(0) > 0, H(0) > 0$, exhibits positivity for all time $t > 0$.

Proof: We assume that the solution (P, W, H) with positive initial condition exists and is unique

From the system of differential equations of the model $(1)-(3)$

From equation (1) we get,

$$\frac{dP}{dt} = E - cPW - aPH$$

$$\frac{dP}{dt} \geq -P(cW + aH)$$

$$P \geq r_1 e^{-(c+a)\delta_{1u} t}$$

Where r_1 is an integration constant

Hence, $P \geq 0$ as $t \to \infty$.

Similarly, from equation (2), we get,

$$\frac{dW}{dt} \geq -W(b + rH + qcP)$$

$$W \geq r_2 e^{-(b+(qc+r)\delta_{1u})t}$$

Where r_2 is an integration constant

Hence, $W \geq 0$ as $t \to \infty$.

From equation (3), we get,

$$\frac{dH}{dt} \geq -H(MaP + h - grW)$$

$$H \geq r_3 e^{-(h+Ma\delta_{1u})t}$$

Where r_3 is an integration constant

Hence, $H > 0$ as $t \to \infty$.

This proves the lemma.

31 Equilibrium points and existence condition

To determine the equilibrium points, the right-hand side of all equations in model (1)-(3) are equated to zero. The following equilibriums points will be obtained from the simplification of the equations

1Initial equilibrium point:$\tilde{E}(0,0,0)$ where $\tilde{P} = 0, \widetilde{W} = 0, \widetilde{H} = 0,$

Therefore, the initial equilibrium

$$(\tilde{P}, \widetilde{W}, \widetilde{H}) = (E, 0,0)$$

2 PFAS free- equilibrium point: $\widehat{E}\,(0, \widehat{W}, \widehat{H})$ where $\widehat{P}$=0, i.e., when PFAS is not present in aquatic ecosystem.

Starting from equation (1), we have

$$\hat{P} = E - cPW - aPH$$

$$\hat{P} = 0$$

We continue with equation (2), we have

$$\widehat{W} = q\widehat{W}(1 - c\hat{P}) - b\widehat{W} - r\widehat{W}\widehat{H}$$

$$H = \frac{b - q}{r}$$

Finally, we take equation (3), we have

$$\widehat{H} = gr\widehat{W}\widehat{H} - Ma\hat{P}\widehat{H} - h\widehat{H}$$

$$W = \frac{h}{gr}$$

Therefore, the pollutant-free equilibrium

$(\hat{P}, \widehat{W}, \widehat{H}) = (E, \frac{b-q}{r}, \frac{h}{gr})$ Will exist if $(b - q) > 0$

3 Interior equilibrium points:$E^*(P^*, W^*, H^*)$: the values of $P^*, W^*, H^*$are given as.

From equation (1) we have,

$$P^* = \frac{q - b - rH^*}{dc}$$

$P^* > 0$ if $(q - b - rH^*) > 0$

$$W^* = \frac{Maq - Mab - MarH^* + hH^*qc}{grqc}$$

$W^* > 0$ if $Maq - Mab - MarH^* + hH^*qc > 0$

H^* is the non-negative real roots of the polynomial equations below,

$$H^{*2}(grq^2c^2ar + hq^2c^3r - Mar^2c^2q)H^*(Marc^2q^2 - hq^3c^3 - Marc^2bq + hd^2c^3b + c^2rMaq^2 - Mabc^2rq - grq^3c^2a + grq^2c^2ab) + (Eq^3c^3gr - Maq^3c^2 + 2Mabc^2q^2 - Mab^2c^2q) = 0$$

From the above equations, there will be at least one non-negative real values if

$$grq^2c^2ar + hq^2c^3r - Mar^2c^2q > 0$$

$$Eq^3c^3gr - Maq^3c^2 + 2Mabc^2q^2 - Mab^2c^2q > 0$$

The dynamical behavior of the model with respect to these equilibrium points in terms of local and global stability will be examined in the following section.

32 Local Stability:

1 For PFAS free- equilibrium point: $\hat{\boldsymbol{E}}(\boldsymbol{0}, \widehat{\boldsymbol{W}}, \widehat{\boldsymbol{H}})$

The variational matrix for system of equation (1)-(3) at PFAS free-equilibrium point $\hat{E}$ is given by

$$\widehat{M} = \begin{bmatrix} Z_1 & 0 & 0 \\ -c\widehat{\boldsymbol{W}}q & Z_2 & Z_5 \\ -Ma\widehat{\boldsymbol{H}} & Z_4 & Z_3 \end{bmatrix}$$

Where,

$$Z_1 = -c\widehat{\boldsymbol{W}} - a\widehat{\boldsymbol{H}}$$

$$Z_2 = q - b - r\widehat{\boldsymbol{H}}$$

$$Z_3 = gr\widehat{\boldsymbol{W}} - h$$

$$Z_4 = gr\widehat{\boldsymbol{W}}$$

$$Z_5 = -r\widehat{\boldsymbol{W}}$$

This is the characteristic equation for the variational matrix $\widehat{M}$is given as:

$$(Z_1 - \lambda)[(Z_2 - \lambda)(Z_3 - \lambda) - Z_4Z_5 = 0$$

The requirements for the equilibrium state $\hat{E}$ to be asymptotically stable according to Routh's Hurwitz criteria are as follows:

$$Z_1 > 0$$

$$Z_2 + Z_3 > 0$$

$$Z_2 + Z_3 > Z_4Z_5$$

i.e.

$$-c\widehat{\boldsymbol{W}} - a\widehat{\boldsymbol{H}} > 0$$

$$q - b - r\widehat{\boldsymbol{H}} + gr\widehat{\boldsymbol{W}} - h > 0$$

$$q - b - r\widehat{\boldsymbol{H}} + gr\widehat{\boldsymbol{W}} - h > -rgf\widehat{\boldsymbol{W}}^2$$

2Interior equilibrium points: $E^*(P^*, W^*, H^*)$

The variational matrix for system of equation (1)-(3) at PFAS free-equilibrium point $\hat{E}$ is given by

$$M^* = \begin{bmatrix} Z_1 & Z_4 & Z_5 \\ Z_7 & Z_2 & Z_6 \\ Z_8 & Z_9 & Z_3 \end{bmatrix}$$

Where,

$Z_1 = -cW^* - a\mathrm{H}^*$

$Z_2 = q - c\mathrm{P}^*q - b - r\mathrm{H}^*$

$Z_3 = grW^* - Ma\mathrm{P}^* - h$

$Z_4 = -c\mathrm{P}^*$

$Z_5 = -a\mathrm{P}*$

$Z_6 = -rW^*$

$Z_7 = -cqW^*$

$Z_8 = -Ma\mathrm{H}^*$

$Z_9 = grW^*$

The characteristic equation corresponding to variational matrix M^* is given as:

$$(Z_1 - \lambda)[(Z_2 - \lambda)(Z_3 - \lambda) - Z_6Z_9] - Z_4[(Z_7Z_3) - Z_6Z_8)] + Z_5[Z_7Z_9 - (Z_2 - \lambda)Z_8] = 0$$

$$(Z_1 - \lambda)[\lambda^2 - \lambda(Z_2 + Z_3 - Z_5Z_8) + (Z_2Z_3 - Z_6Z_9 - Z_3Z_4Z_7 + Z_4Z_6Z_8 + Z_5Z_7Z_9 - Z_2Z_5Z_8 = 0$$

The requirements for the equilibrium state E^* to be asymptotically stable according to Routh's Hurwitz criteria are as follows:

$Z_1 > 0$

$Z_2 + Z_3 > Z_5Z_8$

$Z_2Z_3 + Z_4Z_6Z_8 + Z_5Z_7Z_9 > Z_2Z_5Z_8 + Z_6Z_9 + Z_3Z_4Z_7$

The following requirements must be met for the equilibrium state E* to be stable:

$-cW^* - a\mathrm{H}^* > 0$

$(q - c\mathrm{P}^*q - b - r\mathrm{H}^* + grW^* - Ma\mathrm{P}^* - h) > (-a\mathrm{P}^*)(-Ma\mathrm{H}^*)$

$(q - c\mathrm{P}^*q - b - r\mathrm{H}^*)(grW^* - Ma\mathrm{P}^* - h) + (-cP)(-rW^*)(-Ma\mathrm{H}^*) + (-a\mathrm{P}^*)(-cqW^*)(grW^*) > (q - c\mathrm{P}^*q - b - r\mathrm{H}^*)(-a\mathrm{P}^*)(-Ma\mathrm{H}^*) + (-rW^*)(grW^*) + (grW^* - Ma\mathrm{P}^* - h)(-c\mathrm{P}^*)(-cqW^*)$

4Numerical simulation and sensitivity analysis:

In this section, numerical simulations are carried out to support the analytical results and to assess the impact of some model parameters. Numerical simulation for the model of Equation $(1) - (3)$ is done using MATLAB ODE45. The parameter values are given in Table 1, and the initial conditions

Let us consider the below mentioned value of the model parameters:

Par.	**Description**	**Value**	**Source**
E	Input rate of PFAS	8.585	Estimate
c	Rate at which P is have taken up / consumed by the aquatic population	0.1	Estimate
a	Rate at which PFAS is intake by the human population	0.063	Estimate
q	Natural growth rate of marine population	0.22	Estimate
b	Mortality rate of aquatic Population	0.017	Estimate
h	Natural mortality rate of human population	0.15	Estimate
m	Decrease in human population density due to the consumption of PFAS	0.40001	Estimate
r	Predator eating prey rate	20.4	Estimate
g	Rate of growth of predator upon feeding on prey	0.755	Estimate

The model parameters have been chosen such that the interior equilibrium point E∗ satisfies the conditions of feasibility, boundedness, and stability. Furthermore, for the specified parameter values, the interior equilibrium pointsE^* is observed to be asymptotically stable, and plot the Graph between P (Concentration of PFAS in aquatic body), W (Density of aquatic population), H (Density of human population) and time t with the increasing value of E.

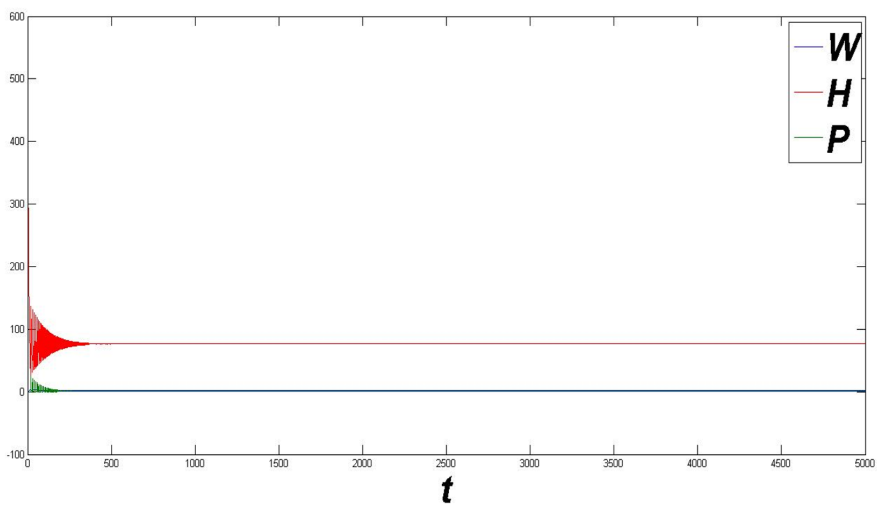

Fig.1.

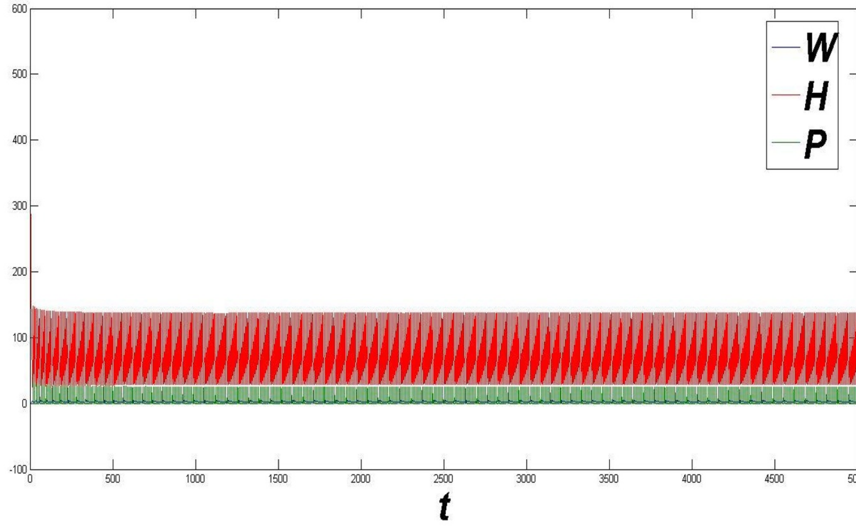

Fig.2.

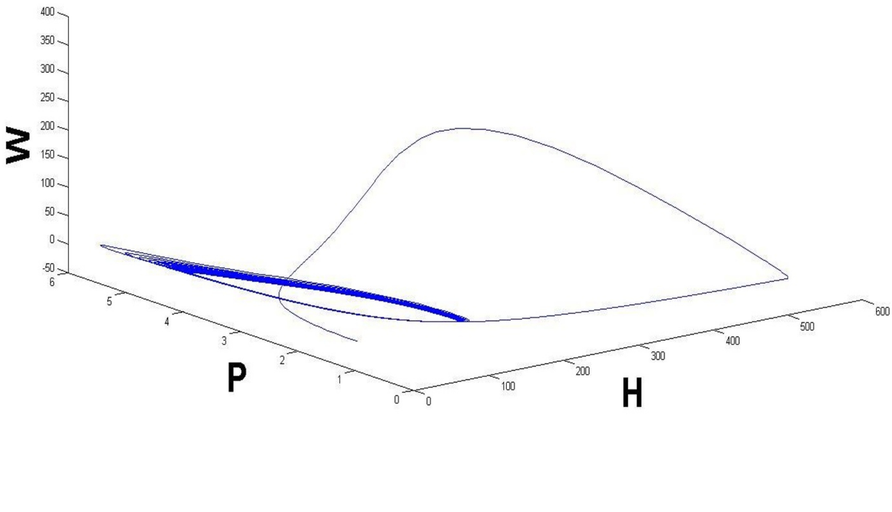

Fig.3.

5 Conclusions

The model is subjected to qualitative analysis as well as numerical simulations.Based on the analysis of the mathematical model given by equations (1)-(3), there isindication that the stability of the system is sensitive to changes in the density of intake rate of PFAS, m. Figure 2 and figure 2, show that increasing the value of ‘m’ beyond a certain threshold leads to an unstable system. Specifically, when 'm' is increased beyond approximately 0.15 to 0.40001, the system becomes unstable and moves away from the equilibrium point. This implies that for the system to be stable the level of PFAS uptake by human population should be maintained bellow 0.40001, thus giving a threshold value to help the scientists and researchers to develop control strategies for PFAS accumulation.

Therefore, it is important to carefully monitor and regulate the intake rate of PFAS to maintain the stability and sustainability of the prey population (W), and predator population (H), as well as the overall ecosystem. This is crucial to prevent any adverse effects on the environment and human health. it is important to take a proactive approach to manage the input rate of PFAS in the environment. As the system is sensitive to changes in the intake rate of PFAS, regulatory bodies need to carefully monitor and control the discharge of PFAS into the environment. This can help to maintain the stability of the ecosystem and prevent any negative environmental and health consequences.

Furthermore, weemphasize the sustainable practices in the use and disposal of PFAS. It is essential to adopt responsible practices to reduce the release of PFAS into the environment. This may include identifying alternative chemicals that are less harmful or implementing more effective treatment methods to remove PFAS from wastewater before discharge.

Overall, we recommend the responsible environmental stewardship and the need for regulations to ensure the sustainability of the ecosystem and human health.

References

1. A. Amin, Z. Sobhani, Y. Liu, R. Dharmaraja, S. Chadalavada, R. Naidu, J.M. Chalker, C. Fang, ETI, **19** (2020).
2. Banyoi, Silvia-Maria, T. Porseryd, J. Larsson, M. Grahn, P. Dinnétz, EP, **315** (2022).
3. C. Beans,PNAS, **118**, (2021).
4. Bell, M. Erin, S. De Guise, J.R. McCutcheon, Y.Lei, M. Levin, B. Li, J.F. Rusling, STE, **780** (2021).
5. Bernardini, Ilaria, V. Matozzo, S.Valsecchi, L.Peruzza, G.D.Rovere, S.Polesello, S. Iori, EI, **152** (2021).
6. Coperchini, Francesca, L. Croce, G. Ricci, F. Magri, M. Rotondi, M. Imbriani, L. Chiovato, FIE, **11** (2021).
7. C. Dora, C. Flores, P.R. Hasselerharm, A.Paraian, J. Caixach, C.M. Villanueva, ISEE, **16** (2021).
8. Garg, Shafali, P. Kumar, V. Mishra, R. Guijt, P. Singh, L.F. Dumée, R.S. Sharma, **38** (2020).
9. Groffen, Thimo, J. Rijnders, L.V. Doorn, C. Jorissen, S.M.D. Borger, D.O. Luttikhuis, L.D. Deyn, A. Covaci, L. Bervoets, ER, **192** (2021).
10. Imir, O. Berk, A.Z. Kaminsky, Q.Y. Zuo, Y.J. Liu, R. Singh, M.J. Spinella, J. Irudayaraj, W.Y. Hu, G.S. Prins, Z.M. Erdogan, Nut, **13** (2021).
11. Johnson, Carly, MHLJ, **42** (2021).
12. Glüge, Juliane, M. Scheringer, I.T. Cousins, J.C. DeWitt, G. Goldenman, D. Herzke, R. Lohmann, C.A. Ng, X. Trier, Z. Wang, ESPI, **12** (2020).
13. Kotlarz, Nadine, J. McCord, D. Collier, C.S. Lea, M. Strynar, A.B. Lindstrom, A.A. Wilkie, EHP, **128** (2020).
14. Kurwadkar, Sudarshan, J. Dane, S.R. Kanel, M.N. Nadagouda, R.W. Cawdrey, B. Ambade, G.C. Struckhoff, R. Wilkin, STTE, **809** (2022).
15. Mahoney, Hannah, Y. Xie, M. Brinkmann, J.P. Giesy, EEH, **1** (2022).
16. Militao, I. Medeiros, FA. Roddick, R. Bergamasco, L. Fan, ECE, **9**(2021).
17. Panieri, Emiliano, K. Baralic, D. Djukic-Cosic, A.B. Djordjevic,L. Saso, Tox, **10**(2022).
18. Fair, A. Patricia, B. Wolf, N.D. White, S.A. Arnott, K. Kannan, R. Karthikraj, J.E. Vena, ER, **171** (2019).
19. Wu, Congyue, M.J. Klemes, B.Trang, W.R. Dichtel, D.E. Helbling, WR, **182** (2020).
20. Sunderland, M. Elsie, X.C. Hu, C. Dassuncao, A.K. Tokranov, C.C. Wagner, J.G. Allen, ESEP, **29**(2019).
21. Kumar, G., Saha, R., Rai, M.K., Thomas, R. and Kim, T.H., 2019. Proof-of-work consensus approach in blockchain technology for cloud and fog computing using maximization-factorization statistics. *IEEE Internet of Things Journal*, *6*(4), pp.6835-6842.
22. Mia, M., Singh, G., Gupta, M.K. and Sharma, V.S., 2018. Influence of Ranque-Hilsch vortex tube and nitrogen gas assisted MQL in precision turning of Al 6061-T6. *Precision Engineering*, *53*, pp.289-299.
23. Bhushan, B., Sahoo, C., Sinha, P. and Khamparia, A., 2021. Unification of Blockchain and Internet of Things (BIoT): requirements, working model, challenges and future directions. *Wireless Networks*, *27*, pp.55-90.
24. Kaur, T., Kaur, B., Bhat, B.H., Kumar, S. and Srivastava, A.K., 2015. Effect of calcination temperature on microstructure, dielectric, magnetic and optical properties of Ba0. 7La0. 3Fe11. 7Co0. 3O19 hexaferrites. *Physica B: Condensed Matter*, *456*, pp.206-212.

25. Masud, M., Gaba, G.S., Alqahtani, S., Muhammad, G., Gupta, B.B., Kumar, P. and Ghoneim, A., 2020. A lightweight and robust secure key establishment protocol for internet of medical things in COVID-19 patients care. *IEEE Internet of Things Journal*, *8*(21), pp.15694-15703.