Data Article

Data on fate and distribution of organophosphate esters in the soil - sediments from Kathmandu Valley, Nepal

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ABSTRACT

Globally, soil and sediments are known as the likely sinks of various organic pollutants, such as organophosphate esters (OPEs). However, the fate of OPEs in soil/sediment matrices is limited in the whole of South Asia, especially if there should be an occurrence of Nepal. This data article elucidates the fate and distribution of OPEs in soil and sediment samples from the capital city of Nepal (Kathmandu). A total of eight different compounds of OPE was measured in soil (N = 19) and sediment (N = 20) samples collected during October 2014. The median concentration and composition of the individual OPE have been discussed. Additionally, health risk exposure due to ingestion and dermal contact of OPE was assessed to mark the endanger of OPE. Moreover, risk quotient (RQ) for fish, Daphnia, and algae was calculated to forecast the risk of OPEs on aquatic organisms.

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1. Data

The concentration data of OPEs in surface soil and sediment samples are given in Table 5 and Table 6, respectively. The health risk exposure of OPEs via soil ingestion and dermal contact has been discussed in Tables 6 and 7, respectively. Table 8–10 describes the ecological risk quotient of OPEs to fish, daphnia, and algae in Bagmati River. Fig. 2 illustrates the site-specific profile of individual OPEs measured in soil and sediment samples. The spatial distribution of OPEs in soil and sediments has been described in Fig. 3.

2. Experimental design, materials, and methods

2.1. Soil sampling

A total of 19 surface soil (0–15 cm depth, vegetation removed) samples were collected at 19 different locations in Kathmandu Valley using stainless steel scoops during 15–25 October 2014 (Table 1). Each soil sample was a composite of 3 sub-samples, which was collected in a radius of 5 m in a different direction. The soil samples were then wrapped in an aluminum foil packed into sealed polythene bags and kept in an ice bag before transporting to the laboratory. Hand gloves were used to avoid contamination during sampling. The soil samples were freeze-dried, ground to powder and sieved through 500 μm sieve and stored at −20 °C until chemical analysis.

2.2. Sediments sampling

Bagmati River, which flows through the capital city Kathmandu was chosen for the collection of sediment samples. About 50g of surface sediment (top 5 cm) samples were collected using pre-cleaned stainless steel scoop at 20 sites along Bagmati River (a stretch of > 27 km), from Gokarneshwor in the
north to Chobhar in the south. Fig. 1 and Table 2 shows the sampling points along the Bagmati River. Different items, like rocks, sticks, mussels, etc. Were removed from the sediment samples and transported to the laboratory keeping in an icebox. Later, all the sediment samples were stored in the refrigerator at \(-20^\circ\)C until chemical analysis. The sediment samples were freeze-dried, ground to fine, sieved through mesh size of 500 µm, and kept in an amber jar until extraction.

2.3. Sample preparation and analysis

Freeze-dried and homogenized soil/sediment samples were spiked with 1000 ng of deuterated tris (2-chloroethyl) phosphate (TCEP-d12) as a recovery standard. Later, they were Soxhlet extracted with dichloromethane (DCM) for 24 h. Copper granules were added to the round bottle flask before extraction to remove the elemental Sulphur present in soils and sediments. Copper granules were prewashed and activated with hydrochloric acid before adding to the container. The sample extract was concentrated by rotary evaporator (Heidolph 4000, Germany) and was solvent exchanged to hexane with a volume of 0.5 mL. The extract was passed through Supelclean Envi Florisil SPE column tubes 6 mL (1g) (SUPELCO, USA) for purification. Before fractionation, Florisil® cartridges were prewashed with

Table 1

| Sample ID | Sampling site location | Lat & Long | Elevation (m) | Period of sampling | Avg temp | Avg wind speed | Avg rainfall | Remarks |
|-----------|------------------------|-----------|---------------|-------------------|----------|----------------|-------------|---------|
| KTM01     | Sanepa                 | 27°41’3.30”N 85°18’3.83”E | 1284 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-traffic area |
| KTM02     | Satdobato chawk        | 27°39’32.02”N 85°19’28.96”E | 1333 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-traffic area |
| KTM03     | Koteswor               | 27°40’43.41”N 85°20’55.70”E | 1310 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | urban - heavy traffic area |
| KTM04     | Baneshwor              | 27°41’20.36”N 85°20’10.28”E | 1308 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-commercial area |
| KTM05     | Mahraiganj             | 27°44’2.16”N 85°19’48.28”E | 1329 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-traffic area |
| KTM06     | Swayambhu              | 27°42’56.72”N 85°17’1.1”E | 1342 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-traffic area |
| KTM07     | Bhimsengola            | 27°42’4.67”N 85°20’24.68”E | 1322 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-commercial area |
| KTM08     | Pashupati              | 27°42’38.74”N 85°20’46”E | 1320 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Hindu pilgrim place |
| KTM09     | Balkumari bridge       | 27°40’23.36”N 85°20’30.92”E | 1291 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-residential area |
| KTM10     | Airport                | 27°42’2.97”N 85°21’18.13”E | 1327 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | airport |
| KTM11     | Tinkune                | 27°41’7.65”N 85°20’55.13”E | 1295 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | urban - heavy traffic area |
| KTM12     | Kalimati               | 27°41’54.88”N 85°17’52.76”E | 1300 | 2014-10-13 | 23.7 °C | 4 m/s | 239 | Urban-commercial area |
| KTM13     | Kalanki                | 27°41’36.44”N 85°16’51.37”E | 1316 | 2014-10-14 | 23.7 °C | 4 m/s | 239 | urban - heavy traffic area |
| KTM14     | Sinamangal             | 27°41’46.46”N 85°21’01.35”E | 1300 | 2014-10-14 | 23.7 °C | 4 m/s | 239 | Urban - proximity to the airport |
| KTM15     | Balazu Industrial area | 27°43’48.17”N 85°18’03.82”E | 1299 | 2014-10-14 | 23.7 °C | 4 m/s | 239 | Urban-industrial area |
| KTM16     | Bagbazar               | 27°42’22.96”N 85°19’08.66”E | 1297 | 2014-10-14 | 23.7 °C | 4 m/s | 239 | Urban-commercial area |
| KTM17     | Dhapasi height         | 27°44’58.87”N 85°19’54.12”E | 1347 | 2014-10-14 | 23.7 °C | 4 m/s | 239 | Urban-residential area |
| KTM18     | Gwarko, Ring Road      | 27°39’58.62”N 85°19’58.79”E | 1299 | 2014-10-14 | 23.7 °C | 4 m/s | 239 | Urban-traffic area |
| KTM19     | Srijana Nagar          | 27°39’57.17”N 85°23’58.75”E | 1351 | 2014-10-14 | 23.7 °C | 4 m/s | 239 | Suburban-residential area |
Table 2
Details about sediment sampling location.

| Sample ID | Sampling site location | Lat & Long           | Sampling period |
|-----------|------------------------|----------------------|-----------------|
| BGS01     | Gokarna                | 27° 43’ 57.66”N 85° 23’ 7.45”E | 2014-10-16      |
| BGS02     | Guheswori              | 27° 42’ 42.32”N 85° 21’ 13.47”E | 2014-10-16      |
| BGS03     | Gaurighat              | 27° 42’ 46.87”N 85° 20’ 59.75”E | 2014-10-16      |
| BGS04     | Pashupati              | 27° 42’ 35.12”N 85° 20’ 55.43”E | 2014-10-16      |
| BGS05     | Tilganga               | 27° 42’ 12.74”N 85° 20’ 59.87”E | 2014-10-16      |
| BGS06     | Sinanamang             | 27° 41’ 56.01”N 85° 20’ 48.24”E | 2014-10-16      |
| BGS07     | Jagriti Nagar          | 27° 41’ 32.84”N 85° 21’ 4.83”E | 2014-10-16      |
| BGS08     | Gairigaon              | 27° 41’ 18.40”N 85° 20’ 53.61”E | 2014-10-16      |
| BGS09     | Tinkune                | 27° 41’ 10.42”N 85° 20’ 37.34”E | 2014-10-16      |
| BGS10     | Sahyogi Nagar          | 27° 40’ 57.79”N 85° 20’ 21.15”E | 2014-10-16      |
| BGS11     | Chhitij Nagar          | 27° 40’ 44.47”N 85° 20’ 4.23”E | 2014-10-17      |
| BGS12     | Shankhmul             | 27° 40’ 30.28”N 85° 19’ 48.37”E | 2014-10-17      |
| BGS13     | Jwagal                | 27° 41’ 10.29”N 85° 19’ 35.14”E | 2014-10-17      |
| BGS14     | Thapathali            | 27° 41’ 22.27”N 85° 18’ 59.37”E | 2014-10-17      |
| BGS15     | Tirpureshwor          | 27° 41’ 31.75”N 85° 18’ 37.38”E | 2014-10-17      |
| BGS16     | Sanepa                | 27° 41’ 34.26”N 85° 18’ 17.52”E | 2014-10-17      |
| BGS17     | Teku Dovan            | 27° 41’ 27.94”N 85° 18’ 7.61”E | 2014-10-17      |
| BGS18     | Balkhu                | 27° 41’ 3.99”N 85° 17’ 58.17”E | 2014-10-17      |
| BGS19     | Sundarighat           | 27° 40’ 28.29”N 85° 17’ 36.35”E | 2014-10-17      |
| BGS20     | Chobhar               | 27° 39’ 28.46”N 85° 17’ 37.04”E | 2014-10-17      |

Table 3
Full name and GS-MS parameter of OPEs.

| Acronym | Full name                                           | CAS No. | Chemical formula | Mol. Wt. | Quantifier/ Qualifier | RT   |
|---------|-----------------------------------------------------|---------|------------------|----------|-----------------------|------|
| TNBP    | Tri-n-butyl phosphate                               | 126-73-8 | C_{13}H_{27}O_{6}P | 266.3    | 155/99                | 7.063|
| TCEP    | Tris (2-chloroethyl)phosphate                        | 115-96-8 | C_{12}H_{24}O_{6}P | 285.5    | 249/143               | 7.696|
| TCIPP-1 | Tris (1-chloro-2-propyl)phosphate (mix of three isomers) | 13674-84-5 | C_{14}H_{28}O_{6}P | 327.6    | 125/277               | 7.877|
| TCIPP-2 |                                                     |         |                  |          |                       |      |
| TCIPP-3 |                                                     |         |                  |          |                       |      |
| TCIPP-4 |                                                     |         |                  |          |                       |      |
| TDCIPP  | Tris (1,3-dichloropropyl)phosphate                   | 13674-87-8 | C_{15}H_{27}Cl_{3}O_{6}P | 430.9    | 191/381               | 12.210|
| TPHP    | Triphenyl phosphate                                 | 115-86-6 | C_{18}H_{15}O_{6}P | 326.3    | 170/228               | 13.107|
| EHDPP   | 2-Ethylhexyl diphenyl phosphate                      | 1241-94-7 | C_{20}H_{22}O_{6}P | 362.4    | 251/170               | 13.329|
| TEHP    | Tri (2-Ethylhexyl)phosphate                         | 78-42-2  | C_{24}H_{30}O_{6}P | 436.4    | 113/211               | 13.592|
| TMPPP-1 | Tri-cresyl phosphate (mix of three isomers)          | 1330-78-5 | C_{21}H_{29}O_{6}P | 368.4    | 243/170               | 16.020|
| TMPPP-2 |                                                     |         |                  |          |                       |      |
| TMPPP-3 |                                                     |         |                  |          |                       |      |
| TCESP   | deuterated tris (2-chloroethyl) phosphate d_{12}      | 1276500- | C_{12}H_{24}O_{6}P | 297.5    | 261/148               | 7.635|
| HMB     | Hexamethylbenzene                                   | 87-85-4  | C_{12}H_{18}      | 162.3    | 162/147               | 6.330|

Table 4
Level of average OPEs and RSD detected in blank samples of soil and sediments.

| OPEs    | Soil blank (ng/g) | Sediments blank (ng/g) |
|---------|-------------------|------------------------|
|         | Lab (n = 10) | RSD (%) | Lab (n = 10) | RSD (%) |
| TNBP    | 4.80   | 1.9    | 4.68   | 1.40   |
| TCEP    | 3.54   | 0.27   | 3.36   | 1.10   |
| TCIPPs  | 4.69   | 0.65   | 4.15   | 0.82   |
| TDCIPP  | 0.48   | 0.01   | 5.84   | 1.48   |
| TPHP    | 5.12   | 2.60   | 1.30   | 0.51   |
| EHDPP   | 9.10   | 2.66   | 1.47   | 0.23   |
| TEHP    | 0.82   | 0.41   | ND     | 0      |
| TMPPS   | 2.17   | 0.16   | 4.35   | 1.40   |
6 mL ethyl acetate, 6 mL hexane/DCM (8:2, v/v), and 10 mL hexane to clean and condition the adsorbent. After the extract was transferred to the SPE column, the first fraction was eluted with 6 mL 8:2 Hex: DCM and was discarded. The second fraction that contained target OPFRs were eluted with 20 ml ethyl acetate, evaporated until dryness under constant nitrogen flow and the residue was redissolved in 200 mL of iso-octane. The resulting fraction was transferred to GC vials for GC-MS analysis. Before GC-MS injection, a known amount (1000 ng) of hexamethyl benzene (HMB) was added as an internal standard for quantification purposes.

2.4. GC-MS analysis

Eight target OPEs (TCEP, TCIPPs: mix of three isomers, TDCIPP, TNBP, TEHP, TPHP, EHDPHP and TMPPs: mix of three isomers) were analyzed using Agilent GC (7890A) coupled with 7000A Triple quadrupole coupled MSD, with a DB5-MS capillary column (30 m × 0.25 mm i. d. × 0.25 μm film thickness). One μL of the sample was injected in splitless mode, and the temperature of the injector was 295 °C. Helium was used as carrier gas at the flow rate of 1 mL min⁻¹. The temperature of the transfer line and ion source was maintained at 280 °C and 230 °C, respectively. The GC oven temperature started at 60 °C for 1 min, increased to 220 °C at a rate of 30 °C min⁻¹ (held for 0 min), then to 300 °C at a rate of 5 °C min⁻¹ (held for 15 min). The full name of eight OPEs is given in Table 3.

2.5. Quality assurance/quality control

Since OPFRs are ubiquitous to the indoor environment, we adopted strict precaution and QA/QC criteria to minimize the contamination. All the glassware was soaked in 5% KOH and 95% ethanol solution and washed with Milli-Q water, followed by DCM and hexane. Then the cleaned glassware was oven-dried and was baked at 450 °C for 6h and rinsing with solvents. Although we took utmost care, it appears that contamination with OPEs may occur at some point in extraction, clean up, or analysis in the laboratory. Hence, we followed a rigorous cleaning procedure before experimentation to ensure minimum contamination of OPEs. We used prebaked Na₂SO₄ as a blank soil/sediment sample, which was packed in aluminum foil and taken to sampling sites and brought back to the laboratory with soil/sediment samples.
Ten laboratories blank each for soil, and sediments were extracted and analyzed together with samples to assess the possible contamination of the samples. The level of OPFRs detected in laboratory blank ranged from 0.48 to 9.10 ng/g and 1.30–5.84 ng/g for soil and sediments, respectively (Table 4). The method detection limits (MDLs) are the mean plus three times the standard deviation of all the blank samples. When the compounds were not detected in the blank, the MDL was calculated as three times signal to noise ratio obtained from the lowest spiked standard. The MDLs of OPFRs ranged from 0.51 to 17.08 ng/g and 2.83–17.52 ng/g in soil and sediments, respectively. The average recovery of the surrogate standard (TCEP-d12) was 108 ± 6.4% and 124 ± 5.2% for soil and sediments, respectively. In this data, the concentrations of target OPFRs were blank corrected, but not corrected for recovery.

### 2.6. Health risk assessment

Soil ingestion and dermal absorption of soil to the general population of Kathmandu were assessed using the health risk assessment model recommended by USEPA and is expressed in the following equations (1) and (2). All the constant factors/parameters used in the health risk assessment model were obtained from the literature [2–4].

#### Table 6
Concentration of OPEs in sediment samples (ng/g).

| Sampling sites | OPE compounds |
|----------------|---------------|
|                | TNBP | TCEP | TCIPPs | TDCIP | TPHP | EHDPHP | TEHP | TMPPs |
| BGS-1          | 5.04 | 16.04 | 54.49 | 4.25 | 47.30 | 117.08 | 1149.72 | 945.30 |
| BGS-2          | 10.23 | 10.96 | 14.67 | 3.89 | 7.92 | 52.11 | 2379.19 | 431.07 |
| BGS-3          | 25.62 | 16.31 | 12.25 | 4.75 | 20.27 | 170.22 | 978.52 | 462.78 |
| BGS-4          | 40.46 | 18.78 | 26.14 | 3.99 | 16.98 | 417.60 | 1151.87 | 982.32 |
| BGS-5          | 11.24 | 11.26 | 1.69 | 5.53 | 3.33 | 37.71 | 1639.89 | 509.45 |
| BGS-6          | 16.87 | 12.94 | 8.71 | 5.33 | 13.06 | 36.74 | 1699.33 | 800.55 |
| BGS-7          | 46.89 | 24.11 | 84.35 | 6.32 | 39.19 | 148.92 | 1004.35 | 2162.37 |
| BGS-8          | 57.40 | 19.90 | 883.48 | 4.98 | 32.05 | 179.12 | 1091.76 | 938.72 |
| BGS-9          | 78.40 | 35.39 | 90.70 | 6.62 | 91.40 | 164.93 | 778.17 | 459.15 |
| BGS-10         | 93.48 | 38.30 | 51.00 | 6.14 | 130.09 | 196.37 | 777.60 | 469.84 |
| BGS-11         | 29.46 | 17.01 | 7.84 | 5.21 | 15.05 | 99.84 | 1713.72 | 1038.28 |
| BGS-12         | 29.83 | 18.60 | 16.84 | 5.96 | 21.16 | 132.16 | 3024.98 | 1334.29 |
| BGS-13         | 239.25 | 17.98 | 218.55 | 8.54 | 129.46 | 158.51 | 703.86 | 1306.01 |
| BGS-14         | 319.39 | 12.81 | 333.32 | 5.41 | 12.35 | 238.99 | 656.50 | 1046.58 |
| BGS-15         | 17.48 | 12.83 | 5.23 | 4.97 | 7.97 | 47.84 | 1970.74 | 548.77 |
| BGS-16         | 39.50 | 16.79 | 22.74 | 4.96 | 19.37 | 58.66 | 2292.37 | 481.95 |
| BGS-17         | 213.23 | 14.61 | 152.45 | 7.45 | 51.71 | 117.72 | 886.32 | 1510.93 |
| BGS-18         | 183.27 | 11.97 | 196.61 | 6.64 | 19.76 | 120.33 | 704.13 | 1074.47 |
| BGS-19         | 16.41 | 13.67 | 15.73 | 4.10 | 5.24 | 33.93 | 1364.76 | 284.58 |
| BGS-20         | 54.26 | 28.91 | 55.00 | 4.47 | 108.19 | 173.93 | 1136.40 | 1629.74 |

#### Table 7
Health risk exposure of OPE via soil ingestion and dermal contact (ng/kg bw/day).

| OPE | Soil ingestion | Dermal absorption via soil | RfD  |
|-----|----------------|----------------------------|------|
| TNBP | 0.005 | 0.040 | 2.4 × 10^4 |
| TCEP | 0.004 | 0.031 | 2.2 × 10^4 |
| TCIPPs | 0.009 | 0.077 | 8.0 × 10^4 |
| TDCIP | 0.005 | 0.046 | 1.5 × 10^4 |
| TPHP | 0.004 | 0.031 | 7.0 × 10^4 |
| EHDPHP | 0.007 | 0.062 | – |
| TEHP | 0.007 | 0.063 | – |
| TMPPs | 0.012 | 0.100 | 1.3 × 10^4 |
| OPE | 0.053 | 0.451 | – |
Soil ingestion exposure \(= \frac{CS \times DI}{BW} \) (1)

Dermal contact via soil \(= \frac{CS \times DAS \times ESA \times AF}{BW} \) (2)

where CS refers level of OPEs in soil (ng/g), DI is daily soil intake (20 mg/day) [2], DAS represents dust adhered to skin rate (0.01mg/cm²) [2–4], while ESA denotes exposed skin area (1000cm²) [2]. AF signifies absorption factor (0.17%) [5].

2.7. Ecological risk assessment

The risk quotient (RQ) approach is widely used to assess the impact of pollutants on non-target aquatic organisms. In this data, sediment-based OPE concentration is utilized to determine the risk of OPE contaminants on aquatic organism recommended by Santos et al. [6] and Sanchez-Avila et al. [7]. The RQs are estimated as a quotient of the observed environmental level and the predicted no-effect concentration.

\[ RQ = \frac{MEC}{PNEC} \] (3)

\[ PNEC = \frac{EC_{50}}{f} \] (4)

where MEC refers to the measured environmental concentration. PNEC denotes the predicted no-effect level and can be calculated as the ratio of the toxicological relevant concentration (EC_{50}) and security factor (f). The EC_{50} for OPE compounds was acquired from the Environmental Risk Limits report for OPEs [8], while 1000 was used as a security factor. The risk was estimated exclusively for those chemicals where EC_{50} is available. In this data, MEC was representing pore water concentration and used instead of the direct measure of OPEs in sediments. We assumed that pore-water is the main route

| Fish   | TNBP | TCEP | TCIPPs | TDCIP | TPHP | TMPPs | ΣOPE  |
|--------|------|------|--------|-------|------|-------|-------|
| BGS-1  | 0.4  | 0.2  | 1.4    | 1.9   | 55.4 | 3562.4| 3621.7|
| BGS-2  | 0.8  | 0.1  | 0.4    | 1.8   | 9.4  | 1639.1| 1651.6|
| BGS-3  | 11.7 | 0.9  | 1.8    | 12.5  | 138.9| 10197.9| 10363.7|
| BGS-4  | 21.2 | 1.2  | 4.4    | 12.0  | 132.9| 24730.1| 24901.7|
| BGS-5  | 0.6  | 0.1  | 0.0    | 1.6   | 2.5  | 1217.9| 1222.6|
| BGS-6  | 0.9  | 0.1  | 0.1    | 2.6   | 9.9  | 1955.1| 1968.7|
| BGS-7  | 2.7  | 0.2  | 1.6    | 2.1   | 34.4 | 6100.6| 6141.6|
| BGS-8  | 3.1  | 0.1  | 15.6   | 1.6   | 26.3 | 2476.6| 2523.3|
| BGS-9  | 2.9  | 0.2  | 1.1    | 1.4   | 51.1 | 826.2 | 883.0 |
| BGS-10 | 3.9  | 0.2  | 0.7    | 1.5   | 82.0 | 952.8 | 1041.2|
| BGS-11 | 5.7  | 0.4  | 0.5    | 5.8   | 43.5 | 9646.9| 9702.8|
| BGS-12 | 6.7  | 0.5  | 1.2    | 7.7   | 71.2 | 14430.8| 14518.1|
| BGS-13 | 7.0  | 0.1  | 2.0    | 1.4   | 56.4 | 1828.8| 1895.7|
| BGS-14 | 16.8 | 0.1  | 5.6    | 1.6   | 9.7  | 2645.5| 2679.4|
| BGS-15 | 2.3  | 0.2  | 0.2    | 3.8   | 15.9 | 3511.1| 3533.5|
| BGS-16 | 5.1  | 0.3  | 0.9    | 3.7   | 37.2 | 2973.7| 3020.8|
| BGS-17 | 6.5  | 0.1  | 1.5    | 1.3   | 23.6 | 2213.8| 2246.7|
| BGS-18 | 9.4  | 0.1  | 3.2    | 2.0   | 15.2 | 2658.8| 2688.7|
| BGS-19 | 2.7  | 0.3  | 0.8    | 3.9   | 13.1 | 2286.9| 2307.7|
| BGS-20 | 10.8 | 0.7  | 3.5    | 5.1   | 321.5| 15577.6| 15919.2|
of exposure for fish, Daphnia, and alga. The pore-water concentration was estimated using the equilibrium partitioning approach suggested by Di Toro et al. [9].

\[
C_{pw} = \frac{C_s}{f_{oc}K_{oc}} \quad (5)
\]

where \(C_{pw}\) represents calculated pore water concentration, \(C_s\) is the concentration of OPEs in sediments (mg/kg), \(f_{oc}\) denotes the content of organic carbon in sediments, and \(K_{oc}\) is the partitioning coefficient of organic carbon in sediment. The degree of ecological risk due to sediment contamination can be estimated based on the magnitude of RQ. The RQ value < 1, denote no significant risk, RQ between 1 and 4 denote moderate risk, between 4 and 20 denote high risk, between 20 and 40 denote very high risk, and > 40 denote extreme risk.

| Table 9 | Estimated Risk quotient (RQ) of different OPEs for Daphnia and total RQ in the Bagmati River. |
|--------|------------------------------------------------------------------------------------------|
| Daphnia | TNBP | TCEP | TCIPPs | TDCIP | TPHP | TMPPs | \(\Sigma\) OPE |
| BGS-1   | 1.5  | 0.0  | 0.5    | 0.5   | 21.2 | 1451.4 | 1475.1 |
| BGS-2   | 3.1  | 0.0  | 0.1    | 0.5   | 3.6  | 667.8  | 675.2  |
| BGS-3   | 45.6 | 0.2  | 0.6    | 3.6   | 53.0 | 4154.7 | 4257.7 |
| BGS-4   | 82.2 | 0.3  | 1.4    | 3.4   | 50.7 | 10075.2| 10213.3|
| BGS-5   | 2.2  | 0.0  | 0.0    | 0.5   | 0.9  | 496.2  | 499.8  |
| BGS-6   | 3.3  | 0.0  | 0.0    | 0.7   | 3.8  | 796.5  | 804.4  |
| BGS-7   | 10.7 | 0.0  | 0.5    | 0.6   | 13.1 | 2485.4 | 2510.4 |
| BGS-8   | 12.2 | 0.0  | 5.1    | 0.4   | 10.0 | 1009.0 | 1036.9 |
| BGS-9   | 11.4 | 0.0  | 0.4    | 0.4   | 19.5 | 336.6  | 368.3  |
| BGS-10  | 15.3 | 0.1  | 0.2    | 0.4   | 31.3 | 388.2  | 435.5  |
| BGS-11  | 22.1 | 0.1  | 0.2    | 1.7   | 16.6 | 3930.2 | 3970.8 |
| BGS-12  | 26.0 | 0.1  | 0.4    | 2.2   | 27.2 | 5879.2 | 5935.1 |
| BGS-13  | 27.0 | 0.0  | 0.7    | 0.4   | 21.5 | 745.1  | 794.7  |
| BGS-14  | 65.3 | 0.0  | 1.9    | 0.5   | 3.7  | 1077.8 | 1149.1 |
| BGS-15  | 9.0  | 0.1  | 0.1    | 1.1   | 6.1  | 1430.4 | 1446.7 |
| BGS-16  | 19.7 | 0.1  | 0.3    | 1.0   | 14.2 | 1211.5 | 1246.8 |
| BGS-17  | 25.2 | 0.0  | 0.5    | 0.4   | 9.0  | 911.9  | 937.0  |
| BGS-18  | 36.6 | 0.0  | 1.1    | 0.6   | 5.8  | 1083.2 | 1127.2 |
| BGS-19  | 10.6 | 0.1  | 0.3    | 1.1   | 5.0  | 931.7  | 948.8  |
| BGS-20  | 41.9 | 0.2  | 1.2    | 1.5   | 122.8| 6346.4 | 6513.8 |

| Table 10 | Estimated Risk quotient (RQ) of different OPEs for algae and total RQ in Bagmati River. |
|----------|--------------------------------------------------------------------------------------|
| Algae    | TNBP | TCEP | TCIPPs | TDCIP | TPHP | TMPPs | \(\Sigma\) OPE |
| BGS-1    | 0.6  | 0.3  | 0.9    | 0.1   | 46.6 | 1351.3 | 1399.7 |
| BGS-2    | 1.3  | 0.2  | 0.2    | 0.1   | 7.9  | 621.7  | 631.4  |
| BGS-3    | 18.4 | 1.6  | 1.2    | 0.4   | 116.7| 3868.2| 4006.4 |
| BGS-4    | 33.3 | 2.1  | 2.9    | 0.4   | 111.6| 9380.4| 9530.6 |
| BGS-5    | 0.9  | 0.1  | 0.0    | 0.0   | 2.1  | 462.0  | 465.1  |
| BGS-6    | 1.3  | 0.1  | 0.1    | 0.1   | 8.3  | 741.6  | 751.6  |
| BGS-7    | 4.3  | 0.3  | 1.1    | 0.1   | 28.9 | 2314.0 | 2348.6 |
| BGS-8    | 4.9  | 0.2  | 10.4   | 0.0   | 22.1 | 939.4  | 977.1  |
| BGS-9    | 4.6  | 0.3  | 0.7    | 0.0   | 43.0 | 313.4  | 362.0  |
| BGS-10   | 6.2  | 0.3  | 0.5    | 0.0   | 68.9 | 361.4  | 437.4  |
| BGS-11   | 8.9  | 0.7  | 0.3    | 0.2   | 36.5 | 3659.2 | 3705.8 |
| BGS-12   | 10.5 | 0.9  | 0.8    | 0.2   | 59.8 | 5473.7 | 5546.0 |
| BGS-13   | 10.9 | 0.1  | 1.4    | 0.0   | 47.3 | 693.7  | 753.5  |
| BGS-14   | 26.4 | 0.1  | 3.7    | 0.1   | 8.2  | 1003.5 | 1042.0 |
| BGS-15   | 3.7  | 0.4  | 0.1    | 0.1   | 13.3 | 1331.8 | 1349.4 |
| BGS-16   | 8.0  | 0.5  | 0.6    | 0.1   | 31.2 | 1228.0 | 1168.3 |
| BGS-17   | 10.2 | 0.1  | 1.0    | 0.0   | 19.8 | 839.7  | 870.8  |
| BGS-18   | 14.8 | 0.1  | 2.2    | 0.1   | 12.8 | 1008.5 | 1038.4 |
| BGS-19   | 4.3  | 0.5  | 0.6    | 0.1   | 11.0 | 867.4  | 883.9  |
| BGS-20   | 16.9 | 1.2  | 2.3    | 0.2   | 270.1| 5908.7| 6199.5  |
Fig. 1. Map of Bagmati river in Kathmandu showing sediment sampling point.

Fig. 2. Site-specific profile of OPE compounds in soil (top) and sediments (bottom) from Kathmandu (adopted from Yadav et al., 2018).
and $< 10$, indicates the small potential for adverse effect, RQ between 10 and $< 100$, specifies considerable potential for adverse effect, and RQ $\geq 100$, suggests potential adverse effect expected.

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**Conflict of Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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