

Occurrence and backtracking of microplastic mass loads including tire wear particles in northern Atlantic air

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Table S1. Summary of marine atmospheric MP data, acquired by active sampling published according to Allen et al., 2022¹ and further literature.

| Reference | Location | MP count [particles m ⁻³] | Size range ^b | Pre- dominant size range ^b | Type of analysis | Polymer composition |
|-----------------------------------|--|--|----------------------------|---|--|--|
| Ding et al., 2021 ² | South China Sea | 0.013 – 0.063 | 50 µm - 2.21 mm | <200 µm | visual, FTIR | Polyester (29%), Rayon (19%), PP (15%), PE (13%), PS (10%) |
| Ding et al., 2022 ³ | Northwestern Pacific Ocean | 0.0046 – 0.064 | 10 – 4556 µm | | µ-FTIR | Rayon (67%), PET (23%) |
| Ferrero et al., 2022 ⁴ | Baltic Sea and Gotland Island | 0 – 85 (301 ^a) | ? µm – 5 mm | 127 µm length 17 µm width | visual, µ-Raman, FTIR | Polyester (39.5%), PC (35.5%), PE (11.8%), PET (5.3%), PU (5.3%) |
| Liu et al., 2019 ⁵ | Western Pacific Ocean (Shanghai – Mariana Islands) | 0 – 1.37 | 20 µm – 2 mm | 318 µm | visual, FTIR | PET (56%), epoxy resin (10%), PE-PP (7%), PS (6%) |
| Trainic et al., 2020 ⁶ | North Atlantic Ocean | 0 – 0.079 | 5 µm – 5 mm | 5 – 10 µm | µ-Raman and visual (confocal microscope) | PS > PE & PP |
| Wang et al., 2020 ⁷ | Pearl River Estuary, South China Sea, Indian Ocean | 0 – 0.077 | 58 – 2252 µm | 851 µm | visual, FTIR | PET (50.0%), PP (22.2%), other (e.g. phenoxy resin, poly(acrylonitrile-co-acrylic acid), poly(ethylene-co propylene) (27.8%) |
| Wang et al., 2021 ⁸ | South China Sea | 0 – 0.013 | 19 – 948 µm | <200 µm | visual, FTIR | PET (54.55%), PMMA (13.64%), EVA (9.09%), PE (9.09%) |

^amax. value detected in the study, with origin from Gdansk Harbour, Poland; ^bNote that in FTIR and Raman spectroscopy studies, MP sizes are typically reported as length in the largest dimension which is different from the concept of the aerodynamic diameter used when sampling PM_{2.5} and PM₁₀ fractions. In order to characterize the MP aerodynamic behavior, both the major and the minor dimensions of the particle are important (e.g. Gonda & Abd El Khalik, 1985⁹).

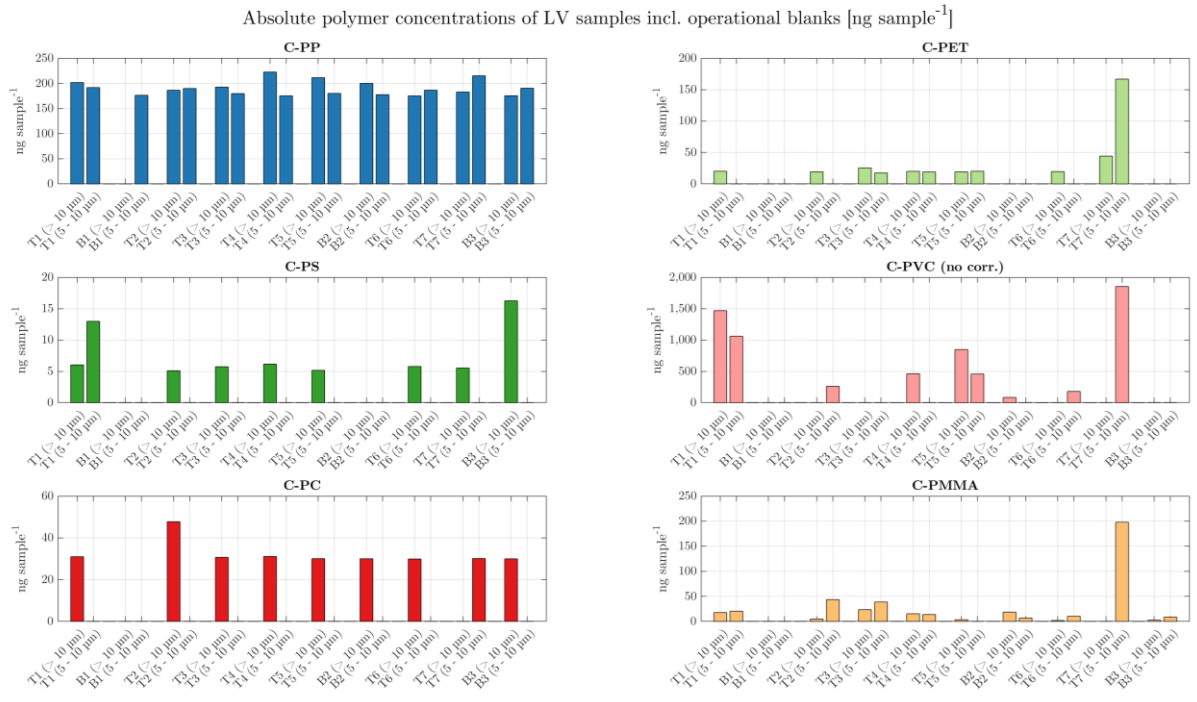


Fig. S1. Absolute polymer concentration ng sample⁻¹ without consideration of total sample volume of the low-volume (LV) samples for transects (T1 – T7) and blanks (B1 – B3). The x-axis reflects the chronological order of sample and blank collection.

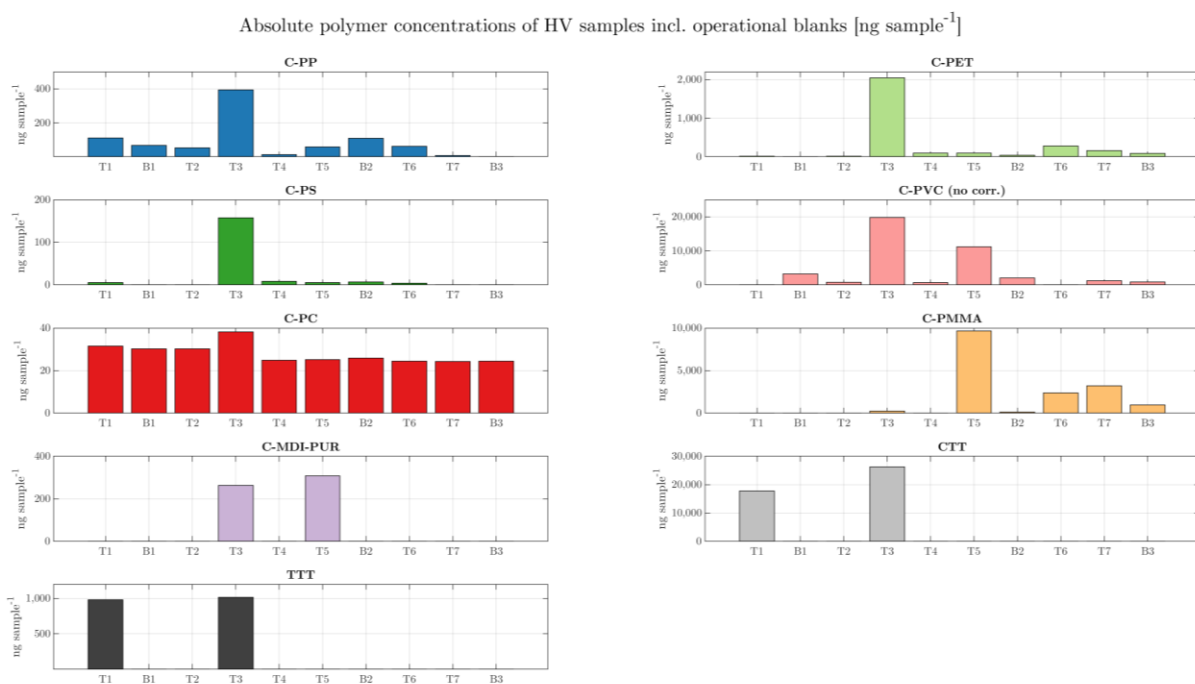


Fig. S2. Absolute polymer concentration ng sample⁻¹ without consideration of total sample volume of the high-volume (HV) samples for transects (T1 – T7) and blanks (B1 – B3). The x-axis reflects the chronological order of sample and blank collection.

Table S2. Limit of detection (LOD) and limit of quantification (LOQ) for respective polymers analysed in this study (*representative for a system in optimum condition).

| Polymer | Limit of detection (LOD) S/N ≥3 (ng absolute*) | Limit of quantification (LOQ) S/N ≥10 (ng absolute*) |
|--------------------|---|---|
| C-PE | 100-300 | 100-300 |
| C-PP | < 100 ^b | 500 |
| C-PET ^a | 10-50 | 50 |
| C-PS ^a | 1 | 2 |
| C-PVC ^a | 10-50 | 50 |
| C-PMMA | < 100 ^b | 100-300 |
| C-PC ^a | 1 | 2 |
| C-MDI-PUR | 100-300 ^b | 500 |
| C-PA6 | 100-300 ^b | 500 |

^abased on dissolved standards; ^bderived from lowest calibration point for orientation only

Table S3. Quantitative results of the low-volume (LV) samplers in ng sample⁻¹ for the 5 -10 µm and > 10 µm size fractions. C-PE and C-PA6 are excluded from the table since they were not detected in any transect nor sampler type.

| | C-PP | C-PET | C-PS | C-PVC | C-PC | C-PMMA | C-MDI-PUR | CTT | TTT |
|-------------------|--------------------------------|-------|------|---------|------|--------|-----------|------|------|
| 5 – 10 µm | ng sample⁻¹ | | | | | | | | |
| T1 | 191.8 | n.d. | 13.0 | 1,059.9 | n.q. | 20.4 | n.d. | n.d. | n.d. |
| B1 | 176.4 | n.d. | n.d. | 0.0 | n.q. | n.q. | n.d. | n.d. | n.d. |
| T2 | 189.8 | n.d. | n.d. | 261.4 | n.q. | 43.6 | n.d. | n.d. | n.d. |
| T3 | 179.8 | 17.4 | n.d. | n.q. | n.q. | 38.7 | n.d. | n.d. | n.d. |
| T4 | 175.3 | 19.1 | n.d. | n.q. | n.q. | 13.7 | n.d. | n.d. | n.d. |
| T5 | 180.2 | 20.2 | n.d. | 456.7 | n.q. | n.q. | n.d. | n.d. | n.d. |
| B2 | 177.7 | n.d. | n.d. | n.q. | n.q. | 6.9 | n.d. | n.d. | n.d. |
| T6 | 186.6 | n.d. | n.d. | 179.6 | n.q. | 10.4 | n.d. | n.d. | n.d. |
| T7 | 215.2 | 166.9 | n.d. | 1,853.0 | 30.1 | 197.8 | n.d. | n.d. | n.d. |
| B3 | 190.5 | n.d. | n.d. | n.q. | n.q. | 8.6 | n.d. | n.d. | n.d. |
| > 10 µm | ng sample⁻¹ | | | | | | | | |
| T1 | 201.7 | 20.2 | 6.0 | 1,468.4 | 31.0 | 17.7 | n.d. | n.d. | n.d. |
| B1 | Not analysed, filter fell down | | | | | | | | |
| T2 | 186.4 | 19.3 | 5.1 | 0.1 | 47.8 | 4.9 | n.d. | n.d. | n.d. |
| T3 | 192.7 | 25.6 | 5.7 | n.q. | 30.7 | 23.4 | n.d. | n.d. | n.d. |
| T4 | 222.6 | 20.0 | 6.2 | 461.9 | 31.1 | 15.3 | n.d. | n.d. | n.d. |
| T5 | 211.4 | 19.3 | 5.2 | 847.6 | 30.0 | 3.4 | n.d. | n.d. | n.d. |
| B2 | 200.2 | n.d. | n.d. | 83.5 | 30.0 | 18.7 | n.d. | n.d. | n.d. |
| T6 | 175.2 | 19.7 | 5.8 | 0.2 | 29.9 | 1.9 | n.d. | n.d. | n.d. |
| T7 | 182.9 | 44.3 | 5.5 | n.q. | n.q. | n.q. | n.d. | n.d. | n.d. |
| B3 | 175.6 | n.d. | 16.3 | n.q. | 30.0 | 2.4 | n.d. | n.d. | n.d. |

n.d. = not detectable; n.q. = not quantifiable

Table S4. Quantitative results of the high-volume (HV) samplers KO and VM and the mean values of the transects T (bold) in ng sample⁻¹ for the > 10 µm size fractions. C-PE and C-PA6 are excluded from the table since they were not detected in any transect nor sampler type.

| | C-PP | C-PET | C-PS | C-PVC | C-PC | C-PMMA | C-MDI-PUR | CTT | TTT |
|-----------|-------------------------|----------------|--------------|-----------------|-------------|----------------|--------------|-----------------|----------------|
| | ng sample ⁻¹ | | | | | | | | |
| KO1 | n.q. | 18.2 | 8.3 | n.q. | 32.6 | n.q. | n.d. | 17,773.8 | 991.7 |
| VM1 | 224.5 | 27.0 | 1.8 | n.q. | 30.5 | n.q. | n.d. | 17,807.6 | 969.9 |
| T1 | 112.2 | 22.6 | 5.1 | n.q. | 31.5 | n.q. | n.d. | 17,790.7 | 980.8 |
| B1 | n.q. | 67.8 | n.q. | n.q. | 30.3 | 30.3 | n.d. | n.d. | n.d. |
| KO2 | 39.9 | 18.0 | n.q. | 1091.4 | 30.0 | n.q. | n.d. | n.d. | n.d. |
| VM2 | 65.6 | 20.7 | 0.4 | 453.8 | 30.3 | n.q. | n.d. | n.d. | n.d. |
| T2 | 52.7 | 19.4 | 0.2 | 772.6 | 30.2 | n.q. | n.d. | n.d. | n.d. |
| KO3 | 449.1 | 3290.5 | 280.8 | 39,523.1 | 49.0 | 501.4 | 525.7 | 33,164.3 | 1,069.1 |
| VM3 | 339.5 | 793.9 | 34.9 | n.q. | 27.3 | n.q. | n.d. | 19,360.7 | 963.5 |
| T3 | 394.3 | 2,042.2 | 157.9 | 19,761.6 | 38.1 | 250.7 | 262.9 | 26,262.5 | 1,016.3 |
| KO4 | 23.0 | 90.2 | 7.6 | 661.7 | 24.8 | n.q. | n.d. | n.d. | n.d. |
| VM4 | 4.7 | 105.2 | 8.6 | 724.8 | 24.8 | n.q. | n.d. | n.d. | n.d. |
| T4 | 13.8 | 97.7 | 8.1 | 693.3 | 24.8 | n.q. | n.d. | n.d. | n.d. |
| KO5 | 59.9 | 119.0 | n.q. | 21680.4 | 24.7 | 19,290.9 | 617.2 | n.d. | n.d. |
| VM5 | 56.9 | 79.9 | 10.7 | 702.1 | 25.5 | n.q. | n.d. | n.d. | n.d. |
| T5 | 58.4 | 99.5 | 5.3 | 1,1191.3 | 25.1 | 9,645.4 | 308.6 | n.d. | n.d. |
| B2 | 110.2 | 45.7 | 6.6 | 2,057.5 | 25.9 | 121.2 | n.d. | n.d. | n.d. |
| KO6 | 13.2 | 108.1 | 0.0 | n.q. | 24.3 | 2064.0 | n.d. | n.d. | n.d. |
| VM6 | 111.5 | 451.4 | 7.5 | n.q. | 24.6 | 2694.3 | n.d. | n.d. | n.d. |
| T6 | 62.4 | 279.8 | 3.7 | n.q. | 24.5 | 2,379.2 | n.d. | n.d. | n.d. |
| KO7 | 0.0 | 104.0 | n.q. | 607.4 | 24.4 | 1,904.3 | n.d. | n.d. | n.d. |
| VM7 | 14.6 | 219.1 | n.q. | 1,896.4 | 24.3 | 4,541.2 | n.d. | n.d. | n.d. |
| T7 | 7.3 | 161.5 | n.q. | 1,251.9 | 24.3 | 3,222.7 | n.d. | n.d. | n.d. |
| B3 | n.q. | 89.8 | n.q. | 885.8 | 24.5 | 958.8 | n.d. | n.d. | n.d. |

n.d. = not detectable; n.q. = not quantifiable

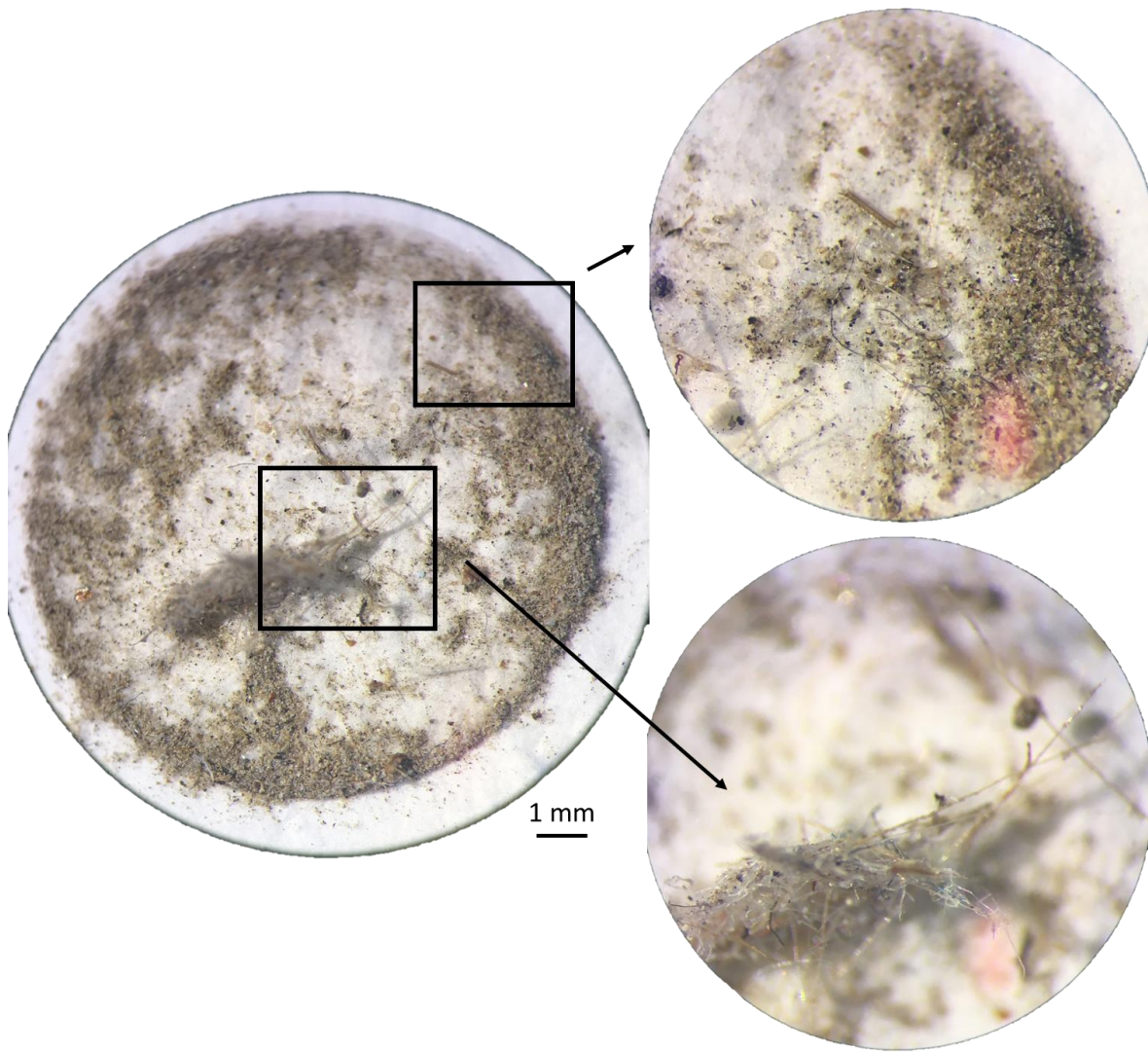


Fig. S3. Filter cake of HV sample KO3 from transect T3 with clearly visible fiber accumulation.

Atmospheric transport and dispersion models

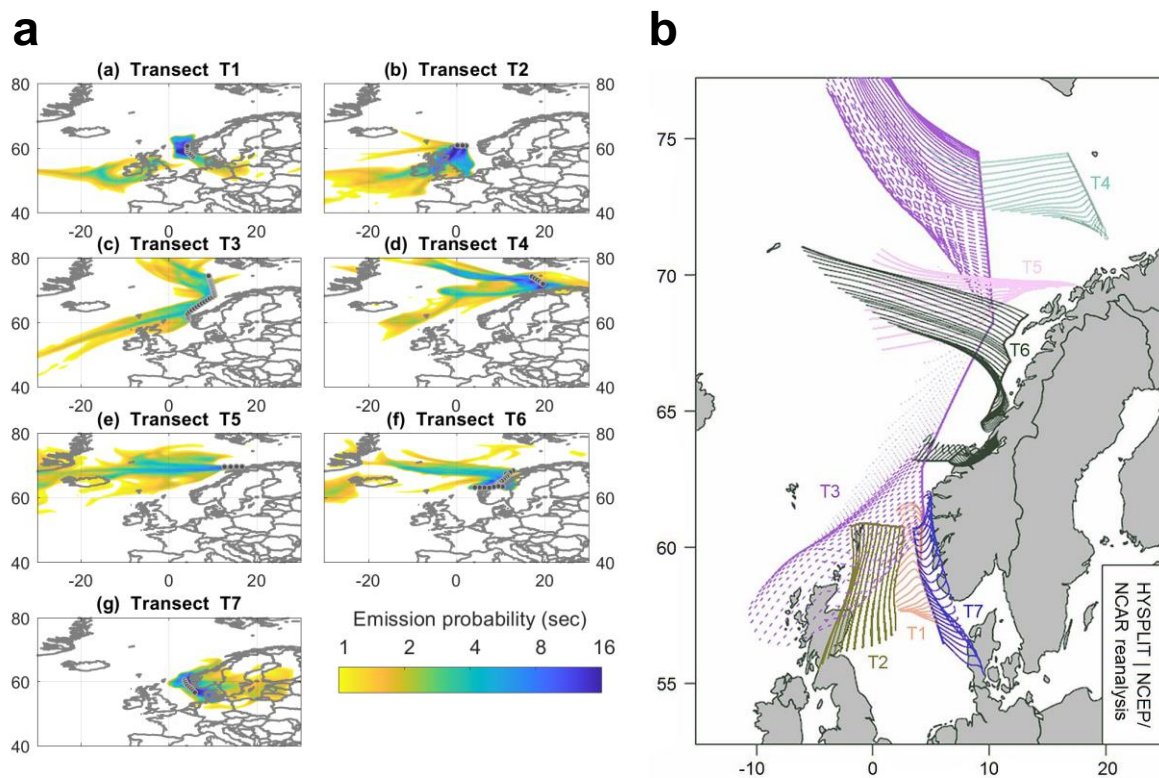


Fig. S4. FLEXPART (FLEXible PARTicle dispersion model) and HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) model results for evaluation of particle and air mass origin for the respective transects, T1 - T7. (a) FLEXPART footprints simulating emissions of microplastic (MP) <math>< 10 \mu\text{m}</math> size fraction at heights from 0 – 100 m above sea level for a duration of 30 days. (b) HYSPLIT back trajectories for the height of 30 m above sea level for a 24-hour duration.

Table S5. Sampling details for the low-volume (LV) sampling.

| Transect | start (in UTC) | End (in UTC) | Start (coordinates) | End (coordinates) | Volume air [m³] |
|-----------------|---------------------------|-------------------------|---------------------------------|---------------------------------|---------------------------------------|
| T1 | 2021-06-06 08:00:00 | 2021-06-07 04:40:00 | 57° 11,705' N 005° 31,688' E | 60° 44,967' N 004° 01,033' E | 92.5 |
| B1 | 2021-06-06 08:00:00 | 2021-06-07 04:40:00 | 57° 11,705' N 005° 31,688' E | 60° 44,967' N 004° 01,033' E | |
| T2 | 2021-06-08 18:00:00 | 2021-06-09 06:00:00 | 60° 45,016' N 002° 38,951' E | 60° 46,176' N 001° 49,459' W | 53.6 |
| T3 | 2021-06-13 11:00:00 | 2021-06-17 06:00:00 | 60° 46,847' N 004° 36,204' E | 74° 31,340' N 008° 59,414' E | 417.0 |
| T4 | 2021-06-20 10:30:00 | 2021-06-21 04:00:00 | 74° 26,573' N 016° 44,146' E | 71° 50,691' N 019° 38,382' E | 78.9 |
| B2 | 2021-06-25 17:09:00 | 2021-06-25 17:10:00 | 69° 38,792' N 017° 17,684' E | 69° 38,792' N 017° 17,684' E | |
| T5 | 2021-06-25 17:10:00 | 2021-06-26 05:25:00 | 69° 38,792' N 017° 17,684' E | 69° 30,100' N 011° 47,634' E | 55.6 |
| T6 | 2021-06-29 12:00:00 | 2021-07-02 03:50:00 | 68° 33,017' N 013° 24,097' E | 63° 11,532' N 003° 22,853' E | 164.4 |
| T7 | 2021-07-04 07:50:00 | 2021-07-05 07:50:00 | 60° 41,173' N 003° 27,712' E | 56° 26,053' N 006° 04,095' E | 108.1 |
| B3 | 2021-07-05 07:50:00 | 2021-07-05 07:51:00 | 56° 26,053' N 006° 04,095' E | 56° 26,053' N 006° 04,095' E | |

Table S6. Sampling details for the high-volume (HV) sampling.

| Transect | Sampler | start (in UTC) | End (in UTC) | Start (coord.) | End (coord.) | Volume air [m³] |
|-----------------------|----------------|---------------------------|-------------------------|------------------------------------|------------------------------------|---------------------------------------|
| T1 | VM1 | 2021-06-06 08:00:00 | 2021-06-07 05:00:00 | 57° 11,705' N 005° 31,688' E | 60° 44,967' N 004° 01,033' E | 504 |
| | KO1 | 2021-06-06 08:00:00 | 2021-06-07 05:00:00 | 57° 11,705' N 005° 31,688' E | 60° 44,967' N 004° 01,033' E | 504 |
| B1 | | 2021-06-07 05:05:00 | 2021-06-07 05:06:00 | 60° 44,967' N 004° 01,033' E | 60° 44,967' N 004° 01,033' E | |
| T2 | VM2 | 2021-06-08 18:00:00 | 2021-06-09 06:00:00 | 60° 45,016' N 002° 38,951' E | 60° 46,176' N 001° 49,459' W | 288 |
| | KO2 | 2021-06-08 18:00:00 | 2021-06-09 06:00:00 | 60° 45,016' N 002° 38,951' E | 60° 46,176' N 001° 49,459' W | 288 |
| T3^a | VM3a | 2021-06-13 11:00:00 | 2021-06-14 11:00:00 | 60° 46,847' N 004° 36,204' E | 64° 39,213' N 006° 02,122' E | 1,728 |
| | VM3b | 2021-06-14 11:00:00 | 2021-06-15 11:00:00 | 64° 39,213' N 006° 02,122' E | 68° 40,381' N 010° 16,242' E | |
| | VM3c | 2021-06-15 11:00:00 | 2021-06-16 11:00:00 | 68° 40,381' N 010° 16,242' E | 72° 23,252' N 009° 30,462' E | |
| | KO3 | 2021-06-13 11:00:00 | 2021-06-17 06:00:00 | 60° 46,847' N 004° 36,204' E | 74° 31,340' N 008° 59,414' E | 2,184 |

| | | | | | | |
|-----------|-----|------------------------|------------------------|------------------------------------|------------------------------------|-------|
| T4 | VM4 | 2021-06-20 10:30:00 | 2021-06-21 03:30:00 | 74° 26,573' N 016° 44,146' E | 71° 50,691' N 019° 38,382' E | 408 |
| | KO4 | 2021-06-20 10:30:00 | 2021-06-21 03:30:00 | 74° 26,573' N 016° 44,146' E | 71° 50,691' N 019° 38,382' E | 408 |
| B2 | | 2021-06-25 17:09:00 | 2021-06-25 17:10:00 | 69° 38,792' N 017° 17,684' E | 69° 38,792' N 017° 17,684' E | |
| T5 | VM5 | 2021-06-25 17:10:00 | 2021-06-26 05:10:00 | 69° 38,792' N 017° 17,684' E | 69° 30,100' N 011° 47,634' E | 288 |
| | KO5 | 2021-06-25 17:10:00 | 2021-06-26 05:10:00 | 69° 38,792' N 017° 17,684' E | 69° 30,100' N 011° 47,634' E | 288 |
| T6 | VM6 | 2021-06-29 12:00:00 | 2021-07-02 03:50:00 | 68° 33,017' N 013° 24,097' E | 63° 11,532' N 003° 22,853' E | 1,532 |
| | KO6 | 2021-06-29 12:00:00 | 2021-07-02 03:50:00 | 68° 33,017' N 013° 24,097' E | 63° 11,532' N 003° 22,853' E | 1,532 |
| T7 | VM7 | 2021-07-04 07:50:00 | 2021-07-05 07:50:00 | 60° 41,173' N 003° 27,712' E | 56° 26,053' N 006° 04,095' E | 576 |
| | KO7 | 2021-07-04 07:50:00 | 2021-07-05 07:50:00 | 60° 41,173' N 003° 27,712' E | 56° 26,053' N 006° 04,095' E | 576 |
| B3 | | 2021-07-05 07:50:00 | 2021-07-05 07:51:00 | 56° 26,053' N 006° 04,095' E | 56° 26,053' N 006° 04,095' E | |

^aDue to technical problems of HV air sampler VM during transect T3, the pre-cleaned aluminum rings were changed two times during sampling. For MP quantification, the lab-blank corrected raw data of the three sub-samples were added up.

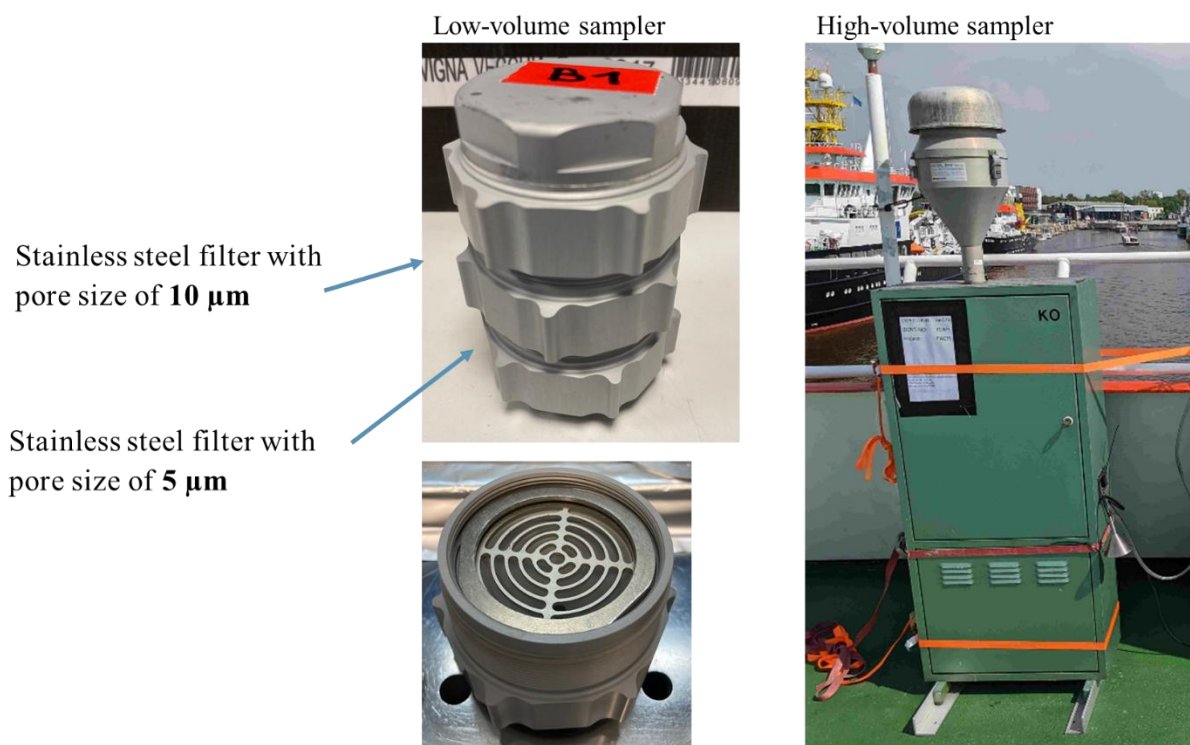


Fig. S5. Pictures of the low- and high-volume sampler.

Table S7. Conditions for Py-GC/MS.

| Micro furnace pyrolyzer & autosampler (EGA/PY-3030D, AS-1020E, (FrontierLabs)) | |
|---|---|
| Carrier gas | Helium |
| Temperature | 590°C |
| Pyrolysis time | 1 min |
| Transfer line temperature | 320°C |
| Gas chromatograph (6890N (Agilent)) | |
| Injector | Split/split less |
| Mode | Split 1:12.5 |
| Temperature | 300°C |
| Pre-column | Trajan P/N 064062; 10 m x 250 µm/363 µm VSDP tubing |
| Column | DB5 (J&W); 30 m x 0.25 mm ID, film thickness 0.25 µm |
| Flow (const.) | 1.2 mL min ⁻¹ |
| Temperature program | 35°C (2 min) → 310°C (30 min) at 4°C min ⁻¹ → hold 60 min |
| Transfer line temperature | 280°C |
| Mass spectrometer (MSD 5973 (Agilent)) | |
| Ionization energy | 70 eV |
| Scan rate | 2.48 scans s ⁻¹ |
| Scan range | <i>m/z</i> 50-650 |
| EI-Source temperature | 230°C |
| Quadrupole temperature | 150°C |

Table S8. Table of characteristic Py-GC/MS composition products used for identification and quantification of detected polymer clusters indicated by “C-“ as pure polymers and potentially included polymer related derivatives according to Goßmann et al., 2022¹⁰.

| Basic polymer cluster | Cluster associated compounds | Characteristic decomposition products | Indicator ions [m/z] |
|-----------------------|---|--|-------------------------------|
| C-PE | HDPE, LDPE, PE-containing copolymers and rubbers, ethylene-vinyl acetate (EVA), EPDM rubber | Alkanes (e.g. C20) | 282 [M], 85 |
| | | α -Alkanes (e.g. C20) | 280 [M], 83 |
| | | α,ω-Alkanes^a (e.g. C20) | 278 [M], 95, 82 |
| C-PP | PP, EPDM rubber | 2,4-Dimethylhept-1-ene | 126 [M], 70 |
| | | 2,4,6,8-Tetramethyl-1-undecene ^b | 210 [M], 100, 69 |
| | | 2,4,6,8-Tetramethyl-1-undecene ^c | 210 [M], 100, 69 |
| | | 2,4,6,8-Tetramethyl-1-undecene ^d | 210 [M], 100, 69 |
| C-PS | PS, PS-containing copolymers (e.g., ABS, SAN), PS- or acryl styrene binders, varnish | Styrene | 104 [M] |
| | | 2,4-Diphenyl-1-butene | 208 [M], 91 |
| | | 2,4,6-Triphenyl-1-hexene | 312 [M], 91 |
| C-PVC | PVC (hard and plasticized), chlorinated rubber | Benzene | 78 [M] |
| | | Chlorobenzene | 112 [M] |
| | | Napthalene | 128 [M] |
| C-PET | PET, polybutylene terephthalate | Dimethyl terephthalate^e | 194 [M], 163 |
| C-PMMA | PMMA; polyalkylated methacrylate, acryl containing binder | Methacrylate | 86 [M], 55 |
| | | Methyl methacrylate | 100 [M], 69 |
| C-PC | PC, epoxide resin | <i>p</i> -Methoxy- <i>tert</i> -butylbenzene ^e | 242 [M], 164, 149 |
| | | 2,2-Bis(4'-methoxy-phenyl)propane^e | 256 [M], 241 |
| C-PA6 | PA6 | ϵ-Caprolactam | 113 [M] |
| | | N-methyl caprolactam^e | 127 [M] |
| C-MDI-PUR | MDI-PUR, MDI-PUR based formulations | 4,4'-Methylenbis(N-methylaniline) ^e | 226 [M] |
| | | N,N-Dimethyl-4-(4-methylamino)benzylanilin ^e | 240 [M] |
| | | 4,4'-Methylenbis(N,N-dimethylaniline)^e | 254 [M], 253, 210, 134 |
| TTT | Truck tire tread, bus tire tread | 2,4-Dimethyl-4-vinylcyclohexene (DMVCH) | 136 [M], 121, 93, 68 |
| | | 1-Methyl-4-(1-methylethenyl)-cyclohexene | 136 [M], 121, 93, 68 |
| CTT | Car tire tread | Ethenylbenzene | 104 [M], 78, 51 |
| | | Cyclohexenylbenzene (SB) | 158 [M], 129, 115, 104 |

[m/z] = mass to charge ratio; [M] = molecular ion; bold = indicator ions used for calibration and quantification; ^aMean of *n*-C₁₆-C₂₆-alkadiens used for quantification of PE. ^bisotactic. ^cheterotactic. ^dsyndiotactic. ^eonly after TMAH treatment.

Table S9. Plastic standards used for quantification.

| Polymer standard | Acronym | Additional information | Supplier |
|---|----------------|--|-------------------------------------|
| Polyamide 6 (K891), Alkulon® K222-D | PA6 | Low viscosity | Ter Hell, GmbH, Hamburg, Germany |
| Polycarbonate, Markoplon 2558 | PC | | Bayer Material, Science |
| Polyethylene, Lupolen 4261 AG UV | HDPE | High density | LyondellBasell |
| Polyethylene terephthalate, NEOPET 80 | PET | | Neogroup |
| Polymethyl methacrylate, PLEXIGLAS® 7N | PMMA | | Plexiglas® |
| Polypropylene, HL508FB | PP | | Borealis |
| Polystyrene, TOTAL PS impact 7240 | PS | High impact PS for extrusion industry | Ter Hell, GmbH, Hamburg, Germany |
| Polystyrene, Styrolution PS 158N/L | PS | Raw material | IINEOS Styrosolution |
| Polyurethane | PUR | MDI-PUR | GEBA GmbH |
| Polyvinylchloride, Vinnolit S3268 | PVC | Hard PVC, raw material | Vinnolit |
| All-season truck tire tread | TTT | | Goodyear Tire & Rubber Company |
| All-season car tire tread | CTT | | Semperit (Continental AG) |

Table S10. Overview of calibration measurements.

| | PE | PP | PET | PS | PVC | PC | PMMA | PA6 | MDI-PUR | CTT | TTT |
|---|----|----------|----------|----------|---------|----------|---------|-----|----------|----------|----------|
| Low-volume samples | | | | | | | | | | | |
| Date of measurement sequence: 21.02.22 | | | | | | | | | | | |
| B | / | -0.05332 | -0.03803 | -0.00436 | 0.01165 | -0.24395 | 0.37917 | / | -0.18625 | / | / |
| Slope | / | 0.32666 | 2.40678 | 1.18516 | 0.04308 | 8.1797 | 0.32929 | / | 0.12031 | / | / |
| r² | / | 0.92801 | 0.98071 | 0.79199 | 0.91577 | 0.96756 | 0.9581 | / | 0.79199 | / | / |
| High-volume samples | | | | | | | | | | | |
| Date of measurement sequence: 21.02.22 | | | | | | | | | | | |
| B | / | + | -0.03803 | 0.00236 | 0.01304 | -0.24395 | 0.29926 | / | -0.17117 | -0.06598 | -0.19719 |
| Slope | / | + | 2.40678 | 0.80346 | 0.04212 | 8.1797 | 0.33749 | / | 0.12545 | 0.0039 | 0.20466 |
| r² | / | + | 0.98071 | 0.98299 | 0.81325 | 0.96756 | 0.92302 | / | 0.84494 | 0.85046 | 0.85684 |
| Date of measurement sequence: 03.03.22 | | | | | | | | | | | |
| B | / | + | -0.0867 | -0.00488 | 0.0096 | -0.21184 | 0.08916 | / | -0.01688 | -0.06627 | -0.19719 |
| Slope | / | + | 2.61034 | 0.99491 | 0.04102 | 8.67124 | 0.61426 | / | 0.05375 | 0.0039 | 0.20466 |
| r² | / | + | 0.92496 | 0.92572 | 0.91309 | 0.98733 | 0.96461 | / | 0.86592 | 0.92807 | 0.85684 |
| Date of measurement sequence: 28.03.22 | | | | | | | | | | | |
| B | / | + | -0.0852 | 0.01204 | 0.02129 | -0.16804 | 0.06868 | / | 0.02272 | / | / |
| Slope | / | + | 1.54062 | 0.92369 | 0.04332 | 6.95696 | 0.57043 | / | 0.03838 | / | / |
| r² | / | + | 0.67752 | 0.94112 | 0.82014 | 0.99002 | 0.97171 | / | 0.66994 | / | / |

B = y-intercept, r² = coefficient of determination, / = not identified in samples and therefore not calibrated, + = 1-Point-calibration

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