**Supplementary material Table 1:** Description of predictor variables included in the final LUR models

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Predictor variable | Pollutant | Mean | SD | Min | 5% | 25% | Median | 75% | 95% | Max |
| trafload\_50 | NOx | 586,308 | 841,295 | 0 | 0 | 29,314 | 91,503 | 750,055 | 2,174,623 | 2,562,487 |
| trafload\_100 | PM2.5abs | 1,961,176 | 2,568,870 | 0 | 0 | 249,432 | 1,218,311 | 2,477,363 | 6,714,870 | 9,777,397 |
| trafloadm\_25 | PM10 | 141,632 | 289,636 | 0 | 0 | 0 | 0 | 62,955 | 864,620 | 889,862 |
| trafloadm\_50 | PNC | 534,408 | 817,094 | 0 | 0 | 0 | 0 | 684,722 | 2,157,786 | 2,225,753 |
| trafloadm\_100 | **O3a** | 1,776,468 | 2,590,972 | 0 | 0 | 0 | 1,001,735 | 2,271,340 | 6,193,628 | 9,777,397 |
| roadl\_50 | PM2.5 | 114.8 | 86.1 | 0 | 0 | 58.6 | 106.3 | 179.2 | 214.4 | 302.4 |
| roadl\_1000 | PM10 | 28,331 | 13,511 | 0 | 1,0528 | 1,4586 | 31,139 | 39,546 | 44,662 | 45,706 |
| roadlm\_100 | PM10, NO2 | 137.9 | 164.5 | 0 | 0 | 0 | 142.0 | 197.6 | 511.5 | 544.0 |
| intdistnearminv2 | PMcoarse | 18.03 | 28.2 | 0.02 | 0.04 | 0.16 | 1.9 | 22.6 | 82.5 | 83.9 |
| abld\_25 | PNC, PM10, PM2.5abs | 198.9 | 210.5 | 0.0 | 0.0 | 10.0 | 120.8 | 336.1 | 511.5 | 675.2 |
| abld\_50 | **O3 a** | 1,313.6 | 903.6 | 0.0 | 137.9 | 550.3 | 1,422.3 | 1,735.6 | 2,379.7 | 3,750.0 |
| nbld\_500 | **O3** | 966.8 | 462.2 | 4.0 | 152.2 | 749.3 | 1,117.5 | 1,262.3 | 1,543.1 | 1,677.0 |
| nbld\_1000 | PM2.5abs | 3,081.9 | 1,747.0 | 6.0 | 390.8 | 1,686.8 | 3,482.0 | 4,175.8 | 5,341.6 | 6,625.0 |
| pop\_300 | **O3 a** | 1,098.1 | 844.0 | 1.0 | 30.5 | 482.3 | 980.2 | 1,528.4 | 2,327.2 | 3,029.3 |
| industry\_300 | PNC, PM10, PMcoarse, PM2.5, NOx | 8.6 | 18.9 | 0.0 | 0.0 | 0.0 | 0.3 | 5.9 | 48.7 | 73.9 |
| industry\_1000 | PM2.5abs, NO2 | 10.5 | 9.9 | 0.0 | 0.0 | 2.2 | 8.3 | 15.4 | 21.6 | 41.8 |
| industry\_5000 | NO2 | 8.3 | 7.0 | 0.5 | 0.5 | 1.7 | 8.1 | 15.2 | 18.6 | 19.1 |
| seminat\_100\_neg | PNC, NOx | -3.5 | 8.7 | -33.5 | -21.6 | -0.7 | 0.0 | 0.0 | 0.0 | 0.0 |
| seminat\_1000\_neg | PM2.5, NO2 | -16.0 | 16.1 | -58.2 | -47.7 | -22.7 | -9.8 | -4.6 | -2.3 | -0.3 |
| urbgreen\_500\_neg | PM10 | -6.2 | 6.5 | -23.6 | -16.0 | -10.6 | -4.2 | -1.6 | 0.0 | 0.0 |
| green\_500\_neg | PNC | -16.1 | 11.3 | -48.4 | -34.0 | -20.7 | -16.3 | -6.5 | -3.1 | -0.4 |
| green\_1000\_neg | PNC, NOx | -22.6 | 14.0 | -59.3 | -50.6 | -26.3 | -18.9 | -12.3 | -8.4 | -8.1 |
| water\_5000\_neg | PM2.5abs | -1.7 | 1.0 | -3.7 | -3.0 | -2.3 | -2.0 | -1.0 | -0.1 | -0.1 |
| tot\_build\_25 | PM2.5 | 85.3 | 28.8 | 0.0 | 30.4 | 87.8 | 100.0 | 100.0 | 100.0 | 100.0 |
| tot\_build\_1000 | PMcoarse | 57.5 | 28.3 | 0.1 | 21.5 | 32.9 | 68.0 | 81.7 | 88.8 | 91.9 |
| elev\_sqrt\_neg | PM2.5, **O3 a** | -21.9 | 0.8 | -23.6 | -22.7 | -22.3 | -22.0 | -21.5 | -20.3 | -20.3 |

See Table 1 for a detailed explanation of the variable names. Variables with \_X (e.g. trafload\_50) are buffers with \_X indicating the radius of the buffer in meters. The suffix ”\_neg” indicates predictors with a negative sign.

aPredictor variable was multiplied by –1 for the marked pollutant.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Supplementary material Table 2.** Comparison between newly developed LUR models for the area of Augsburg for PM10, PMcoarse, PM2.5, PM2.5absorbance, NOx and NO2 and ESCAPE models**.** | | | | | | | |
|  |  |  |  |  |  |  |  |
| Pollutant | N | LUR model | R² | Adj R² | LOOCV R2 | LOOCV Adj R2 | Moran’s I (p-value) |
| PM10 | 20 | 13.67 + 0.0078 \* roadlm\_100 + 0.000079 \* roadl\_1000 + 0.044 \* industry\_300 + 0.098 \* urbgreen\_500\_neg + 0.0022 \* abld\_25 + 0.0000016 \* trafloadm\_25 | 0.91 | 0.87 | 0.78 | 0.76 | -0.18 (0.15) |
| PM10 ESCAPE | 20 | 18.47 + 0.039 \* roadlm\_50 + 0.57 \* natural\_100\_negc + 0.021 \* roadl\_50 | 0.83 | 0.80 | 0.75 | 0.73 | -0.08 (0.82) |
| PMcoarsea | 19 | 168.7 + 0.031 \* tot\_build\_1000 + 0.030 \* intdistnearminv2 + 0.025 \* industry\_300 + 0.000037 \* xcoord\_neg | 0.75 | 0.68 | 0.57 | 0.55 | -0.11 (0.60) |
| PMcoarse ESCAPE | 20 | 4.09 + 0.025 \* roadlm\_50 + 0.0000042 \* pop\_5000 + 0.012 \* roadl\_50 | 0.81 | 0.78 | 0.69 | 0.67 | -0.15 (0.36) |
| PM2.5 | 20 | 19.47 + 0.0099 \* roadl\_50 + 0.041 \* seminat\_1000\_neg + 0.41 \* elev\_sqrt\_neg + 0.0094 \* tot\_build\_25 + 0.012 \* industry\_300 | 0.84 | 0.79 | 0.70 | 0.69 | -0.12 (0.49) |
| PM2.5 ESCAPE | 20 | 11.9 + 0.019 \* roadlm\_50 + 0.000495 \* roadl\_300 + 0.14 \* urbgreen\_5000\_neg + 0.0000000074 \* trafloadm\_1000 | 0.78 | 0.72 | 0.62 | 0.60 | -0.13 (0.49) |
| PM2.5absb | 19 | −14.07 +0.000000037 \* trafload\_100 + 0.00047 \* abld\_25 + 0.0087 \* industry\_1000 + 0.000058 \* nbld\_1000 + 0.040 \* water\_5000\_neg + 0.0000034 \* xcoord | 0.93 | 0.89 | 0.84 | 0.83 | -0.14 (0.37) |
| PM2.5abs ESCAPE | 20 | 1.34 + 0.000000177 \* trafload\_50 + 0.0018 \* roadl\_50 + 0.000216 \* trafloadm\_1000 | 0.91 | 0.89 | 0.82 | 0.81 | -0.19 (0.21) |
| NO2b | 19 | 12.57 + 0.22 \* industry\_5000 + 0.015 \* roadlm\_100 + 0.10 \* seminat\_1000\_neg + 0.15 \* industry\_1000 | 0.95 | 0.94 | 0.90 | 0.89 | -0.10 (0.64) |
| NO2 ESCAPE | 40 | 7.432 + 0.0000020 \* trafload\_50 + 0.0014 \* intdistnearminv + 0.024 \* roadl\_50 + 0.000015 \* pop\_5000 + 0.041 \* roadlm\_50 + 0.098 \* hldres\_500 | 0.86 | 0.83 | 0.67 | 0.66 | -0.04 (0.86) |
| NOx | 20 | 28.06 + 0.0000084 \* trafload\_50 + 0.27 \* green\_1000\_neg + 0.20 \* industry\_300 + 0.25 \* seminat\_100\_neg | 0.91 | 0.89 | 0.83 | 0.82 | -0.05 (0.94) |
| NOx ESCAPE | 40 | 13.34 + 0.0000039 \* trafload\_50 + 0.0897 \* roadlm\_50 + 0.0038 \* intdistnearminv + 0.000000025 \* trafload\_1000 + 0.051 \* roadl\_50 + 0.195 \* hldres\_1000 | 0.88 | 0.85 | 0.76 | 0.76 | -0.05 (0.65) |
| aWithout rural site 4 (see Figure 1). | | |  |  |  |  |  |
| bWithout traffic site 20 (see Figure 1).  cSum of predictors seminat\_100 and water\_100. | | |  |  |  |  |  |

**Supplementary material Figure 1.** Scatter plots of measured and predicted concentrations together with linear regression lines (one monitor excluded for each PMcoarse, PM2.5abs and NO2).

