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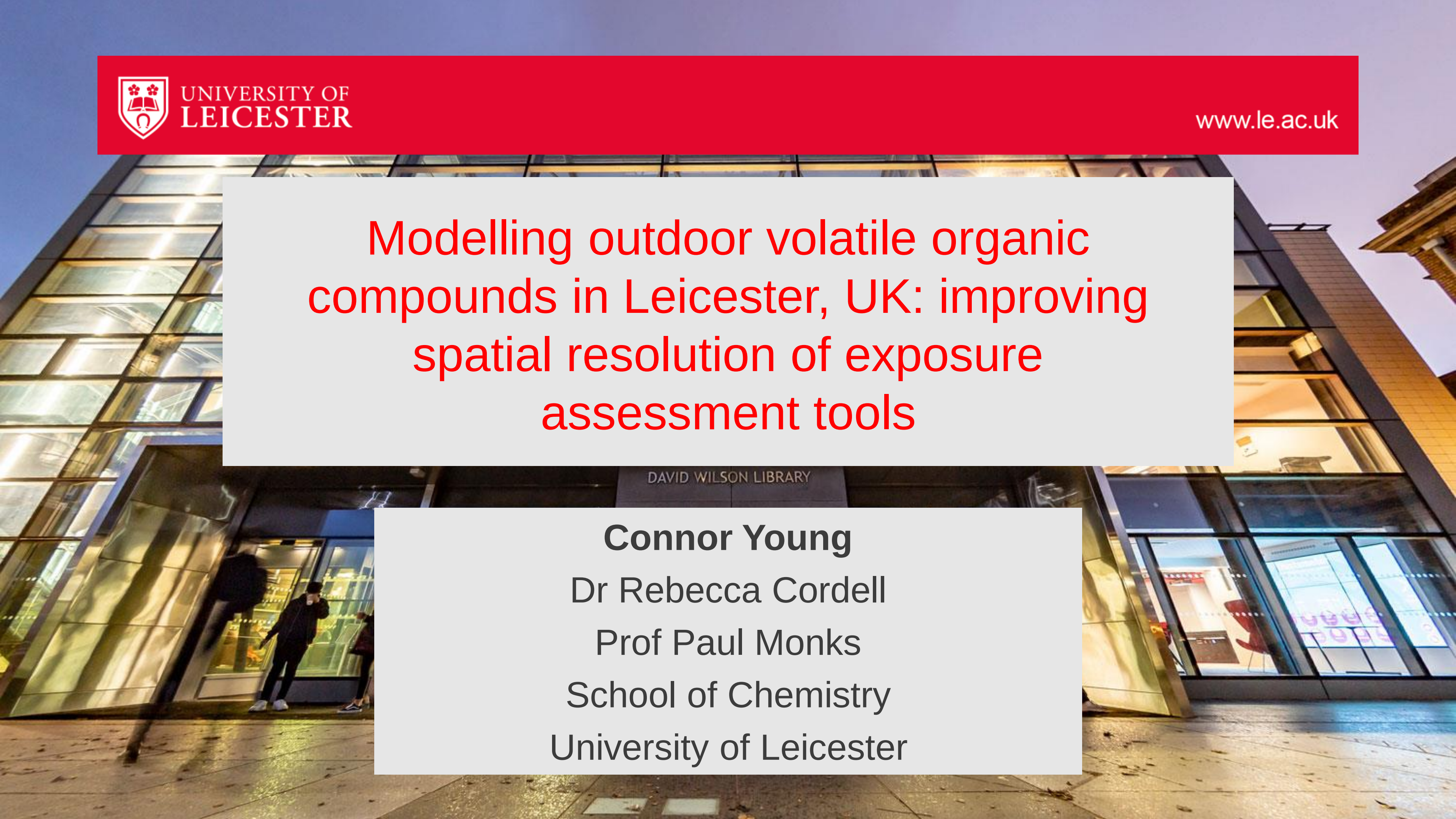
# Modelling outdoor volatile organic compounds in Leicester, UK: improving spatial resolution of exposure assessment tools

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# Why volatile organic compounds (VOCs)?

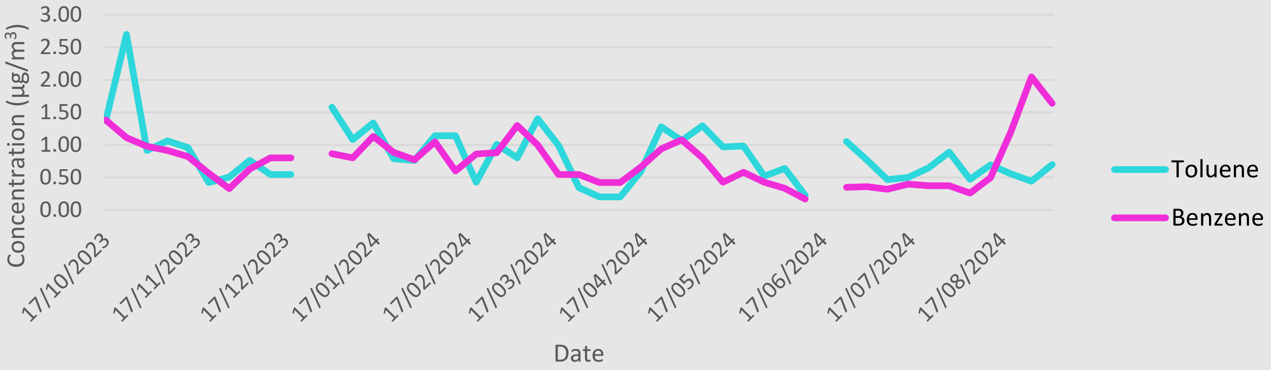
Emitted from anthropogenic and biogenic sources, ubiquitous in outdoor and indoor environments.

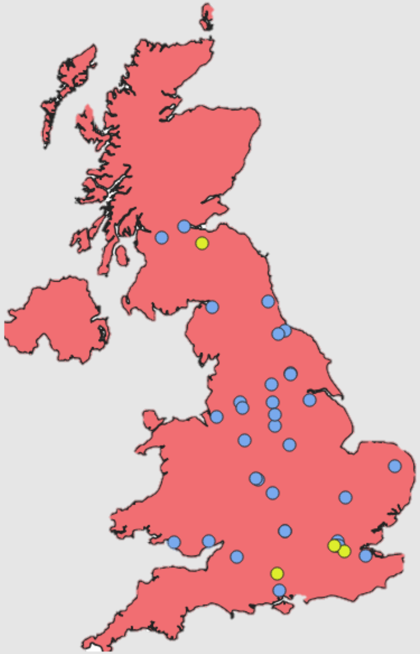
Benzene, toluene, ethylbenzene, and xylene (BTEX) are common outdoor VOCs with known sources.

BTEX are proven carcinogenic hazards and public health concerns.

# Regulation and monitoring

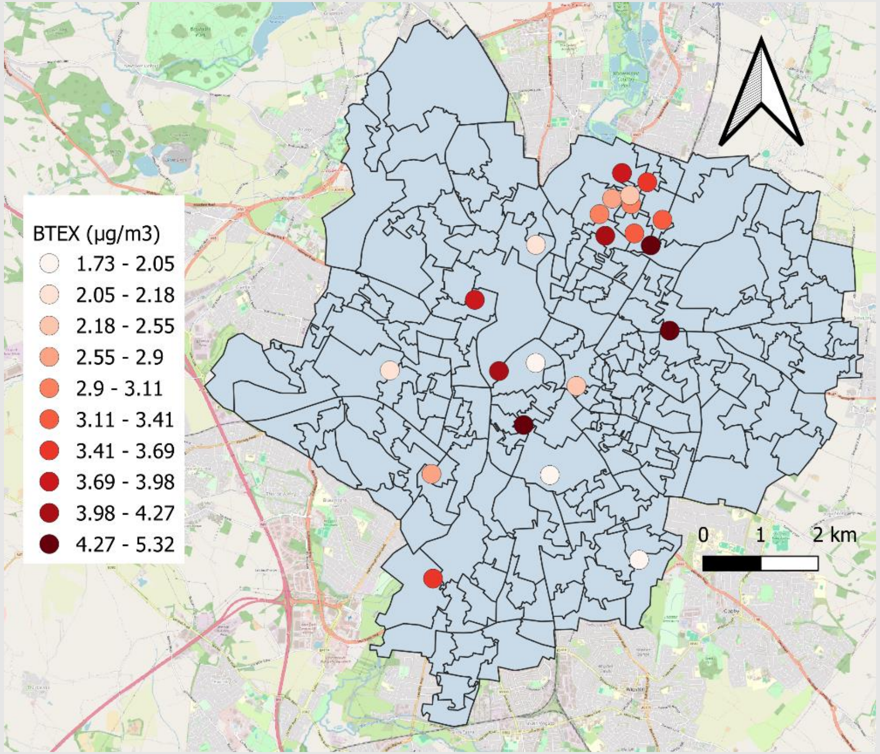
- Ambient outdoor benzene annual average legal threshold: **5 µg/m³**
- Data availability: 4 sites in automatic and 20 in non-automatic UK hydrocarbon networks
- VOC sensors and monitors measure select few compounds or TVOC
- Relatively low ambient outdoor concentrations



# Methodology

- 22 sampling sites across Leicester
- Winter and summer 6-week campaigns (Jan-Feb & Aug-Sep 2024)
- TD-GC-MS analysis
- Weekly passive sampling
- New insight into intra-urban and seasonal variation
- Input data for land-use regression modelling



# Co-location with EarthSense Zephyrs

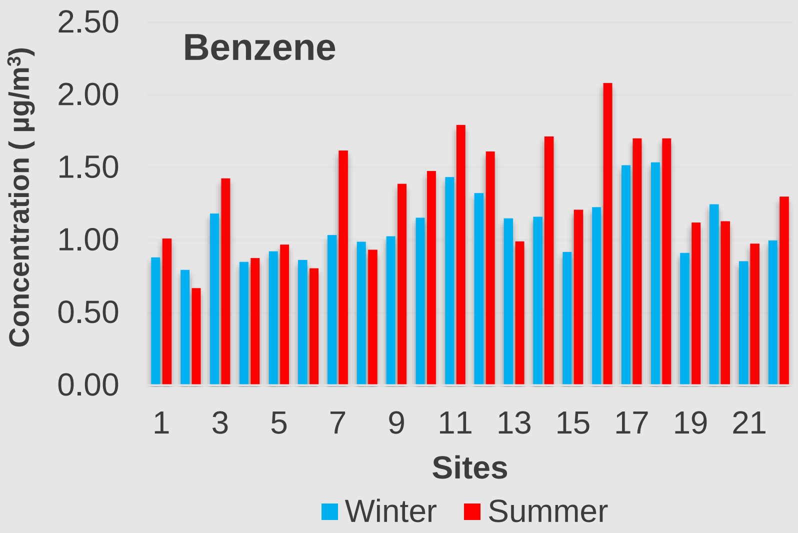
- Higher $NO_2$ and PM on average in Winter
- Lower temperatures related to higher $NO_2$, PM, and BTEX
- Higher $O_3$ related to lower BTEX
- $NO_2$, PM, and BTEX likely co-emission

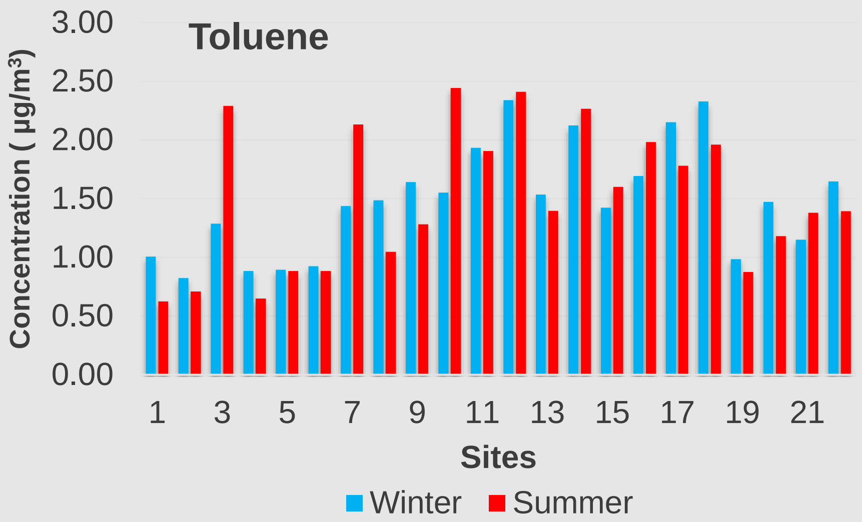
| Date | Temp (°C) | Relative Humidity (%) | $NO_2$ (µg/m³) | $O_3$ (µg/m³) | $PM_{2.5}$ (µg/m³) | $PM_{10}$ (µg/m³) | BTEX (µg/m³) |
|---|---|---|---|---|---|---|---|
| 16/01/2024 | 3.2 | 69.3 | 24.4 | 19.4 | 8.9 | 13.7 | 5.1 |
| 23/01/2024 | 9.6 | 72.8 | 15.1 | 31.7 | 4.2 | 7.8 | 2.7 |
| 30/01/2024 | 9.8 | 78.1 | 17.4 | 23.9 | 6.8 | 11.4 | 2.8 |
| 06/02/2024 | 9.0 | 80.6 | 17.3 | 17.6 | 5.7 | 10.1 | 3.1 |
| 13/02/2024 | 12.5 | 79.7 | 16.8 | 23.7 | 3.4 | 6.7 | 1.9 |
| 20/02/2024 | 8.7 | 76.5 | 18.8 | 27.1 | 5.7 | 9.8 | 2.9 |

| | Temp (°C) | Relative Humidity (%) | $NO_2$ (µg/m³) | $O_3$ (µg/m³) | $PM_{2.5}$ (µg/m³) | $PM_{10}$ (µg/m³) | benzene (µg/m³) | toluene (µg/m³) | ethylbenzene (µg/m³) | p-xylene (µg/m³) | btex (µg/m³) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Winter | 8.8 | 75.8 | 18.3 | 25.1 | 5.9 | 10.2 | 1.1 | 1.5 | 0.3 | 0.4 | 2.9 |
| Summer | 21.4 | 59.3 | 14.5 | 30.7 | 5.2 | 8.1 | 0.9 | 1.8 | 0.2 | 0.2 | 3.1 |

# Intra-urban seasonal variation

- Seasonal changes to BTEX varied across sites
- Concentrations measured at each site influenced by local emission sources rather than regional transport and seasonal meteorological conditions



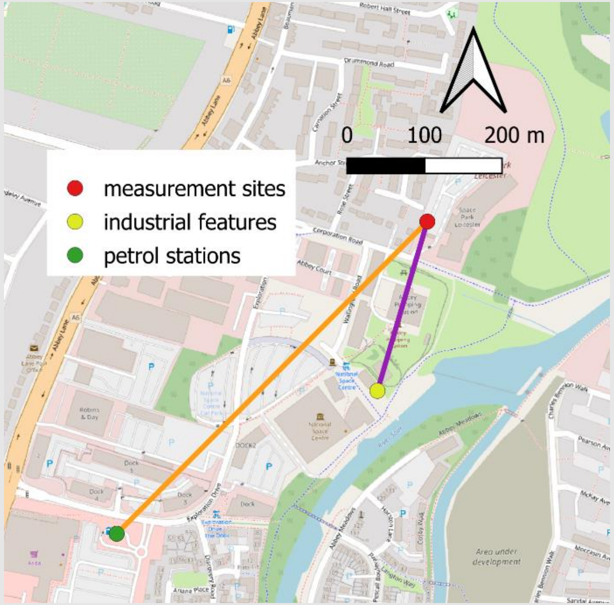
# Intra-urban seasonal variation

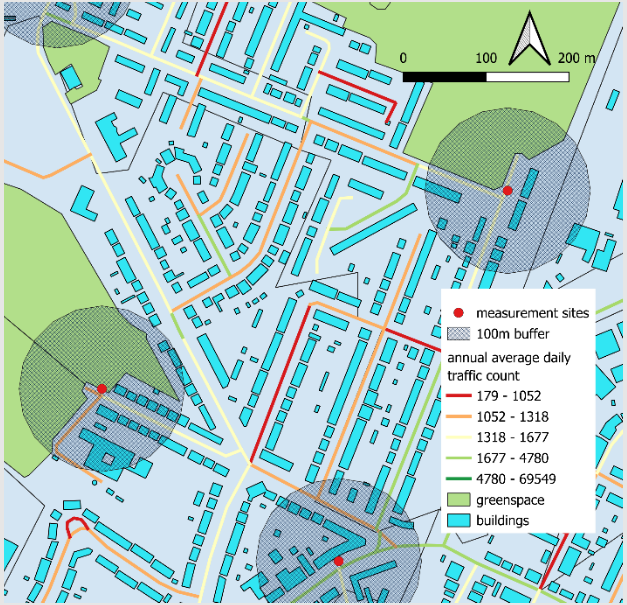
- Higher toluene:benzene indicates more localised, fresh emission sources.
- Ratio around 0.5 suggests dominant road sources, whilst ratios greater than 4 suggests industrial point sources.
- Seasonal variation within Leicester with dominant road sources.

| Site | winter | summer | higher local emissions |
|---|---|---|---|
| 1 | 1.14 | 0.62 | winter |
| 2 | 1.04 | 1.06 | summer |
| 3 | 1.09 | 1.61 | summer |
| 4 | 1.04 | 0.74 | winter |
| 5 | 0.97 | 0.91 | summer |
| 6 | 1.07 | 1.10 | summer |
| 7 | 1.39 | 1.32 | summer |
| 8 | 1.50 | 1.12 | summer |
| 9 | 1.60 | 0.92 | winter |
| 10 | 1.34 | 1.66 | summer |
| 11 | 1.35 | 1.06 | summer |
| 12 | 1.77 | 1.50 | summer |
| 13 | 1.34 | 1.41 | summer |
| 14 | 1.83 | 1.32 | summer |
| 15 | 1.55 | 1.32 | winter |
| 16 | 1.38 | 0.95 | winter |
| 17 | 1.42 | 1.05 | summer |
| 18 | 1.52 | 1.15 | summer |
| 19 | 1.08 | 0.78 | winter |
| 20 | 1.18 | 1.04 | summer |
| 21 | 1.35 | 1.41 | summer |
| 22 | 1.65 | 1.07 | summer |

# Improving the spatial resolution

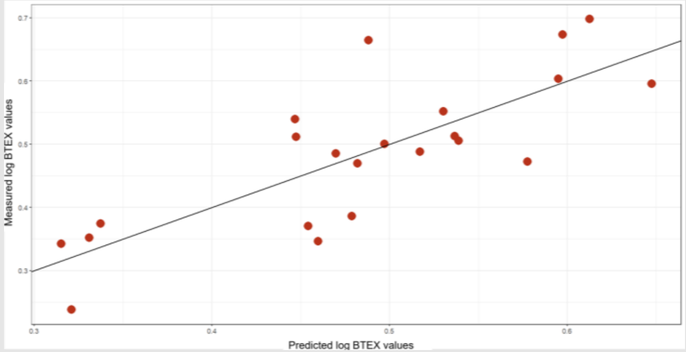
- Land-use regression modelling
- Measured BTEX as input data
- Predictor variables of known geographical source features
- Measured vs Predicted as validation
- Novel approach for VOCs within the UK



# Model selection and performance

- Univariate regression for each predictor
- Selection based on strength of relationship and significance
- Validated by predicting at measured sites
- Comparable to existing VOC LUR models in the literature

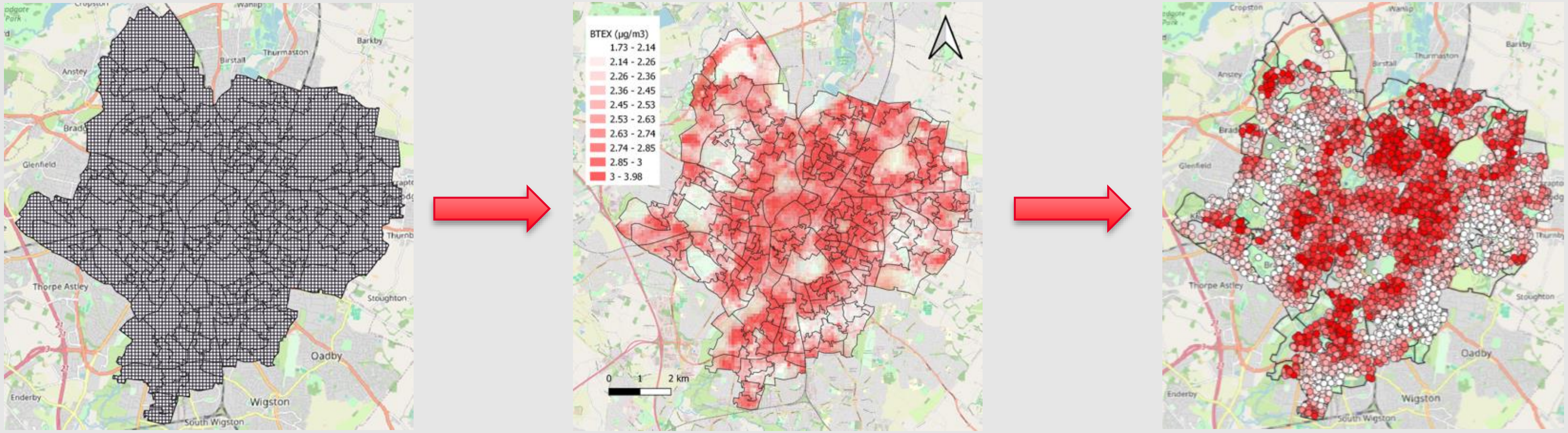



| Predictor variables | $R^2$ | p-value |
|---|---|---|
| Buildings (count within 100 m buffer) | 0.28 | 0.01 |
| Industrial point source (distance to nearest) | 0.35 | 0.004 |
| Elevation | 0.27 | 0.01 |
| Road length (within 100 m buffer) | 0.22 | 0.03 |

| Performance test | BTEX model |
|---|---|
| $R^2$ | 0.63 |
| 4-fold cross validation ($R^2$) | 0.60 |
| LOOCV [a] ($R^2$) (RMSE [b]) | (0.45) (1.17) |
| Moran I (p-value) | -0.086 (0.73) |

# Prediction surfaces for health/social assessments

- 100 m$^2$ resolution (7640 predictions)
- Suitable for post-code level assessment (5589 postcodes)
- ONS individual-level health and social data



# Conclusions

- BTEX concentrations show intra-urban and seasonal variation in Leicester
- Concentrations are related to other primary pollutants ($NO_x$ and PM), but below legal limits
- Land-use regression modelling can effectively improve spatial resolution
- Valuable methodology for more accurate exposure assessments related to health and social outcomes