QUICKSTART GUIDE: HADES

MANUSCRIPT TITLE

Development and evaluation of rapid, national-scale outdoor air pollution modelling and exposure assessment: Hybrid Air Dispersion Exposure System (HADES).

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Data Requirements

- Receptor locations (XY-Points)
- Topography surface
- Building footprints
- Digital elevation model (DEM) surface
- Weather station observations
- Long-range chemical transport model (CTM)
- WorldPop population density surface (100m x 100m records)
- Emission inventory with contributions by SNAP sector (XY-Points and 1km x 1km records)
- Road network

Optional Data

- Building footprints with height attributes
- Road network with modelled annual average daily traffic (AADT) counts
- Area, point, and traffic source activity profiles by time-of-day

Preliminary Model Development

- Develop a database of source specific (area, line, and point) dispersion kernel matrices, for urban and rural locations, under all possible combinations of atmospheric conditions. The plume model equations are found in section 2.2.4 of the main manuscript, with additional parameters found in appendices 12-14.

- The dispersion kernel database should consider 2,016 unique atmospheric combinations, which are based on 7 Pasquill-Turner stability classes, 36 wind direction bands (by 10° increments), and across 8 wind speed groups (1, 2, 3, 4, 6, 8, 10, and 12 m/s). These kernels quantify how NOx concentrations at a central location are influenced by any nearby pollution source within a set search radius. The kernel matrices have a 10m x 10m resolution, and extend from the central location by 500m, 2km, and 4km for road-transport, area, and point sources, respectively.

Fundamental Modelling Environment (FUME)

1. Convert the XY receptor points to a 10m x 10m raster surface.

2. Combine and convert the topography and building footprints to a 10m x 10m simplified primary land use raster surface, using the thematic classifications for a temperate climate found in section 2.1.1 of the main manuscript.

3. Convert the building footprints to a 10m x 10m raster surface that records the average building height within each cell. If building heights are not available, then create a synthetic height dataset using the approach in appendix 2.

4. Using the hourly weather station observations, calculate the average temperature and relative humidity for the time period of interest at each station. Further guidance is provided in section 2.1.3 of the main manuscript.

5. Calculate the 'Urban Index' on the WorldPop 100m x 100m population density surface for your study location. Guidance is provided in section 2.1.5 of the main manuscript, and appendices 1 and 24.

6. Use 'Inverse Distance Weighting' (IDW) to resample the following datasets to 10m x 10m raster surfaces (where required):
    - Ground elevation recorded as the height above sea level (input = DEM).
    - Temperature (input = step 4)
    - Relative humidity (input = step 4)
    - Urban Index (input = step 5)
    - Satellite informed long-range NO_2 contributions (input = CTM)
    - Satellite informed long-range O_3 contributions (input = CTM)

7. Use Focal Statistics to create the following variables that capture the influence of surrounding spatial features (further guidance is provided in appendix 2):
    - Local ground elevation contrast within 1km
    - Ground elevation relative to the national average
    - Greenspace cover within 50m
    - Building cover within 100m
    - Average building height within 100m
    - Standard deviation of the building heights within 100m

8. Apply the upper and lower-level threshold values to the variables calculated in steps 6-7, and apply any necessary transformations (refer to the main manuscript and appendix 2).

9. Resample the 1km x 1km emission inventory records by SNAP sector to the 10m x 10m raster surface created in step 2, using land use informed cell disaggregation. Appendix 3 provides details of this procedure, and an alternative approach to create synthetic data where spatial records are missing.

10. Create a 'total area source' emission surface by summing the area source emission surfaces created in step 9 (excluding SNAP sector 7 which covers road-transport). Convert from tonnes-per-year to cell release rates measured in grams-per-second.

11. Convert the XY point sources (industrial stacks) from the emission inventory to a 10m x 10m raster surface. Convert from tonnes-per-year to cell release rates measured in grams-per-second.

Sequentially Profiled Airshed Release Kernels (SPARK)

12. Temporally scale the annual average 'area' (step 10) and 'point' source (step 11) emission surfaces, using source specific activity profiles by time-of-day (or any other period of interest). Use the profiles provided in appendix 6 if local information is not available. By default, HADES constructs 'hourly-annual average' emission surfaces (n=24).

13. Create the 10m x 10m annual average road-transport emission surface, using one of following approaches listed in descending order of quality:
    - Join the modelled road-traffic data to the road network, and use the HADES traffic toolkit workbook (supplementary file) to disaggregate the spatially resolved AADT counts into 206 vehicle categories, based on spatiotemporal fuel type, emission standard, engine capacity, and age profiles in Great Britain. These profiles may also be used to inform the composition of vehicle fleets in other countries. Apply the vehicle specific COPERT-5 emission functions from the toolkit, accounting for road speed and gradient. Finally, aggregate the 'line' source contributions into a 10m x 10m raster surface with release rates recorded in grams-per-second. Further details of this approach are found in section 2.2.2 of the main manuscript.
    - If modelled AADT counts are not available, then these can be simulated using an OpenStreetMap road network and traffic counts on major roads (see Morley and Gulliver 2016).
    - In locations with sparse data, assign a NOx emissions rate found in appendix 8 to each OpenStreetMap road link and convert the road network to a 10m x 10m raster surface. Then resample the 1km x 1km SNAP sector 7 emission inventory data, using land use informed cell disaggregation with said surface.

14. Temporally scale the annual average 'road' (step 13) emission surface, using source specific activity profiles by time-of-day (or any other period of interest). Use the profile provided in appendix 7 if local information is not available.

15. Convert the hourly measurement data recorded at each weather station, into crosstabulation profiles of wind speed, direction, and stability for the time period of interest (i.e., hourly-annual, seasonal, monthly, or weekly). See section 2.2.3 of the main manuscript for further details. By default, HADES constructs 'hourly-annual average' profiles (n=24).

16. The meteorology profiles created in step 15 are then applied to the dispersion database, to create a series of weighted-average urban and rural source specific kernels for the location and time period of interest (see appendices 15-17).

17. To model the local dispersion processes of road-transport emissions, HADES implements a sequentially profiled airshed release kernels (SPARK) procedure:
    - Divide the study area into a series of 1km x 1km "airsheds", each containing 100 receptor cells;
    - Locate the three nearest weather stations to the centroid point of an airshed;
    - Use IDW to calculate the geographic influence of each physical weather station on the airshed (i.e., triangulation to create a pseudo weather station).
    - Create a time series of weighted-average dispersion kernels for a specified pollutant source in built-up (Urban Index = 1), and rural (Urban Index = 0) locations;
    - Apply the convolution kernels (created in step 16) to the hourly emission surfaces (created in step 13). Then using the Urban Index fraction recorded at each location (created in steps 5-6), weight the time-series of urban and rural exposure surfaces.

18. Repeat step 17 for the 'Area' and then the 'Point' source emission surfaces.

<u>Field Informed Regression Estimates (FIRE)</u>

19. Calibrate the road-transport NO_X concentrations (created in step 17) using the model parameters in appendix 18.

20. Sum the 'Area' and 'Point' source contributions (created in step 18), and calibrate the concentration using the model parameters in appendix 19.

21. Run the calibration model in appendix 20 to calculate the total (all source) NOx concentration at 1m above ground-level.

22. Calculate NO_2 and O_3 concentrations at 1m above ground-level using appendices 21-22.

Dataset Recommendation, Access and Availability

Dataset	Option	Product	Metadata	
Topography	1	Ordnance Survey MasterMap (OSMM)	Spatial Resolution Spatial Coverage Temporal Coverage Access	Polygon vectors (< 1m) Great Britain: Complete Sub-Annual: 2001 to 2024 Restricted: Research, Education, or Licensed
	2	OpenStreetMap (OSM)	Spatial Resolution Spatial Coverage Temporal Coverage Access	Polygon vectors (> 1m) Global: Location Dependent Sub-Annual: Location Dependent Open
	3	CORINE Land Cover (CLC)	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (100m) Europe: Complete Annual: 2000, 2006, 2012, 2018 Open
Digital Elevation Model (DEM)	1	European Environment Agency EU-DEM v1.1	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (25m) Europe: Complete 2011 Open
	2	National Aeronautics and Space Administration (NASA) NASA-DEM 22.04.2021	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (30m) Global: Complete 2000 Open
Building footprints with height attributes	1	Ordnance Survey MasterMap (OSMM)	Spatial Resolution Spatial Coverage Temporal Coverage Access	Polygon vectors (< 1m) Great Britain: Complete Sub-Annual: 2017 to 2024 Restricted: Research, Education, or Licensed
	2	Urban Atlas	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (10m) Europe: Location Dependent 2012 Open

Dataset	Option	Product	Metadata	
Building footprints with height attributes	3	Google Open Buildings 2.5D	Spatial Resolution Spatial Coverage Temporal Coverage Access	Polygon vectors (> 1m) Global: Location Dependent Annual: Location Dependent, 2016 to 2023 Open
	4	Microsoft Planetary Computer (Bing Maps)	Spatial Resolution Spatial Coverage Temporal Coverage Access	Polygon vectors (> 1m) Global: Location Dependent Annual: Location Dependent, 2014 to 2024 Open
Meteorology	1	National Oceanic and Atmospheric Administration Integrated Surface Database (NOAA-ISD)	Spatial Resolution Spatial Coverage Temporal Coverage Access	XY-Points Global: >14,000 active weather stations Hourly: Location Dependent, 1901 to 2024 Open
	2	Copernicus Atmosphere Monitoring Service (CAMS) ERA5-Land model	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (9km) Global: Complete Hourly: 1950 to 2024 Open
Satellite informed Chemical Transport Model (CTM)	1	Copernicus Atmosphere Monitoring Service (CAMS)	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (10km) Europe: Complete Hourly: 1913 to 2023 Open
	2	NASA MODIS	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (1km) Global: Complete 8-Hourly: 2003 to 2023 Open
Demography	1	WorldPop Population Density	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (100m) Global: Complete Annual: 2000 to 2020 Open

Dataset	Option	Product	Metadata	
Emission inventory *	1	National Atmospheric Emission Inventory	Spatial Resolution Spatial Coverage Temporal Coverage Access	Raster surface (1km) Global: Location Dependent Annual: Location Dependent Open (UK)
Road network	1	Ordnance Survey Open Roads	Spatial Resolution Spatial Coverage Temporal Coverage Access	Line vectors Great Britain: Complete Sub-Annual: 2010 to 2024 Open
	2	OpenStreetMap (OSM)	Spatial Resolution Spatial Coverage Temporal Coverage Access	Line vectors Global: Location Dependent Sub-Annual: Location Dependent Open

* All European countries are required to have a 1x1km national atmospheric emission inventory to meet their regulatory compliance with the European Monitoring and Evaluation Programme (EMEP) and the United Nations Framework Convention on Climate Change (UNFCCC).