A study of cooking and cleaning activities with the MBM-Flex indoor air quality model

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Outline

The IAQ-EMS project

- Indoor Air Quality–Emissions and Modelling System: the project aims to improve our understanding of indoor air pollutants, their formation and health effects.
- Project components:
  1. compilation of an **Indoor Pollutant Inventory**.
  2. measurements of key pollutants in representative indoor spaces: residential homes, offices, schools.
  3. development of chemical mechanisms for indoor models.
  4. a large eddy simulation model with simplified chemistry (**Chem-LES**): intra-room dynamics, ventilation effects, pollutants hotspots.
  5. a multi-box model with detailed chemistry (**MBM-Flex**): inter-room dynamics, emissions and evolution of pollutants, human exposure.

MBM-Flex model

- Designed to model air quality in buildings with multiple interconnected rooms.
- The core of MBM-Flex is the **INCHEM-Py** indoor chemistry box-model:
  1. Master Chemical Mechanism (MCM).
  2. additional gas-phase chemical mechanism (BVOCs, OVOCs, chlorine).
  3. photolysis rates corrected for indoor conditions and a range of lighting types.
  4. gas-particle partitioning for α-pinene, β-pinene, limonene.
  5. indoor emissions and deposition of gas-phase species and particles ($PM_{2.5}$).
  6. indoor-outdoor exchange.

MBM-Flex architecture

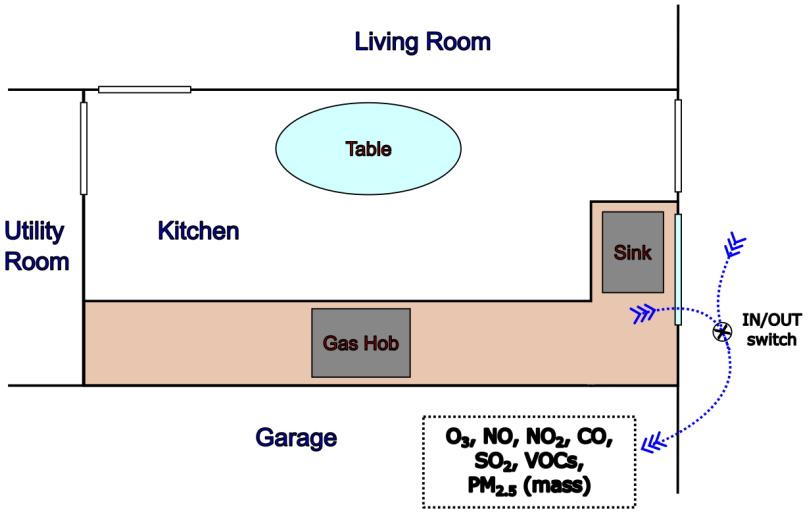
MBM-Flex is designed as a series of communicating INCHEM-Py instances, each representing one room of the building.

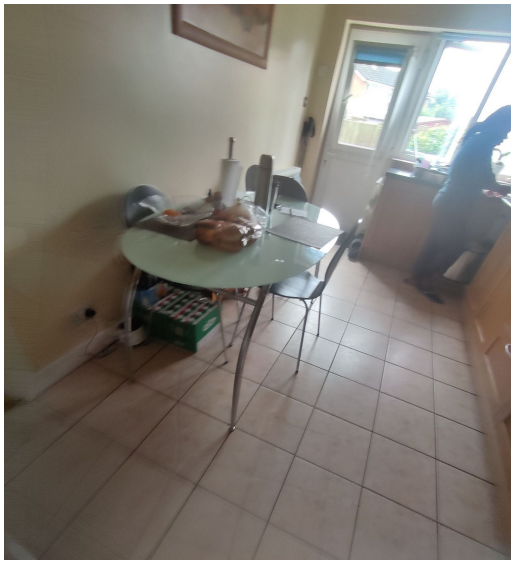
MBM-Flex setup

- Modified version of INCHEM-Py v1.2:
  1. humidity dependent parametrization for HONO emissions from NO_2 reaction on surfaces.
  2. capability to use subsets of the MCM or reduced/lumped chemical mechanisms.
  3. hourly variation of humidity, room occupancy (number of adults and children), indoor-outdoor exchange rate, indoor lighting.
- Each INCHEM-Py instance is configured separately: room dimensions, types of surfaces and lighting, number of people, emissions from various activities, etc...
- Inter-room transport and indoor-outdoor ventilation connect the various INCHEM-Py instances
  $\rightarrow$ informed by Chem-LES model simulations.

Fieldwork in a residential home

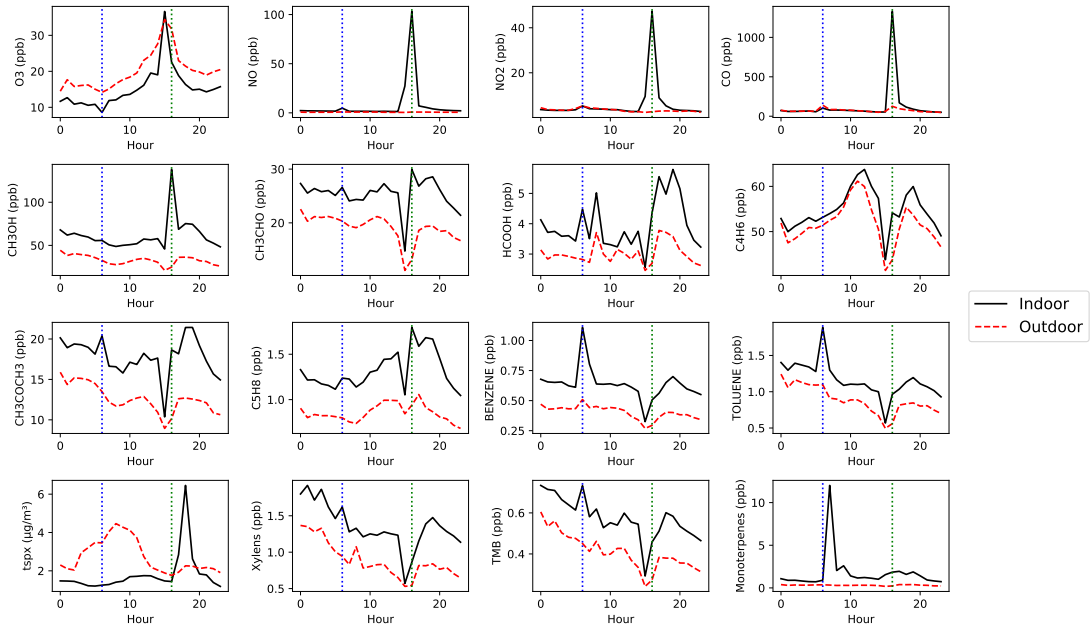
- Measurements in a suburban home southeast of Birmingham (UK) during August 2023.
- A suite of instruments measured a range of gas-phase species and particles – volunteers asked to keep an activity log.
- Sampling switched between indoor and outdoor every 30 minutes.





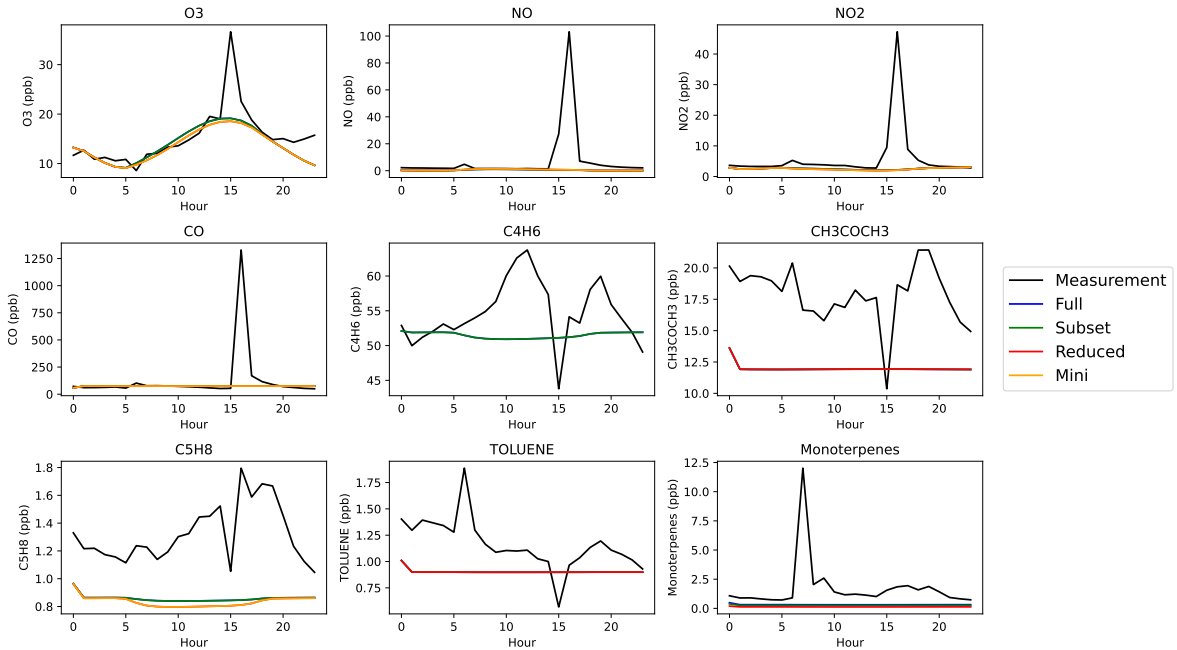
Kitchen measurements

- Focus on 17th August – a case study for kitchen related activities: human presence, cooking and cleaning.
- Two events: 6:00-8:00 and 15:00-18:00, with 1-2 people present and the external door window open.
- Markers of kitchen activity: NO_x, CO (gas hob), acetone (human breath), monoterpenes (food and/or fragrances).



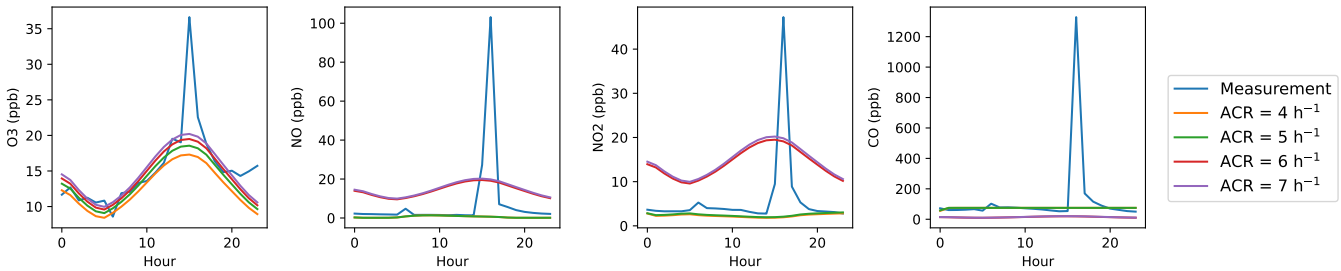
Model setup & results

- Model constrained to the diurnal profile of outdoor O_3, NO_x, CO and initialized with average values for all other parameters.
- **Base case**: no occupants, no kitchen activities.
- Four chemical mechanisms of different complexity:
  ↪ from >18k ("Full") to <150 ("Mini") reactions



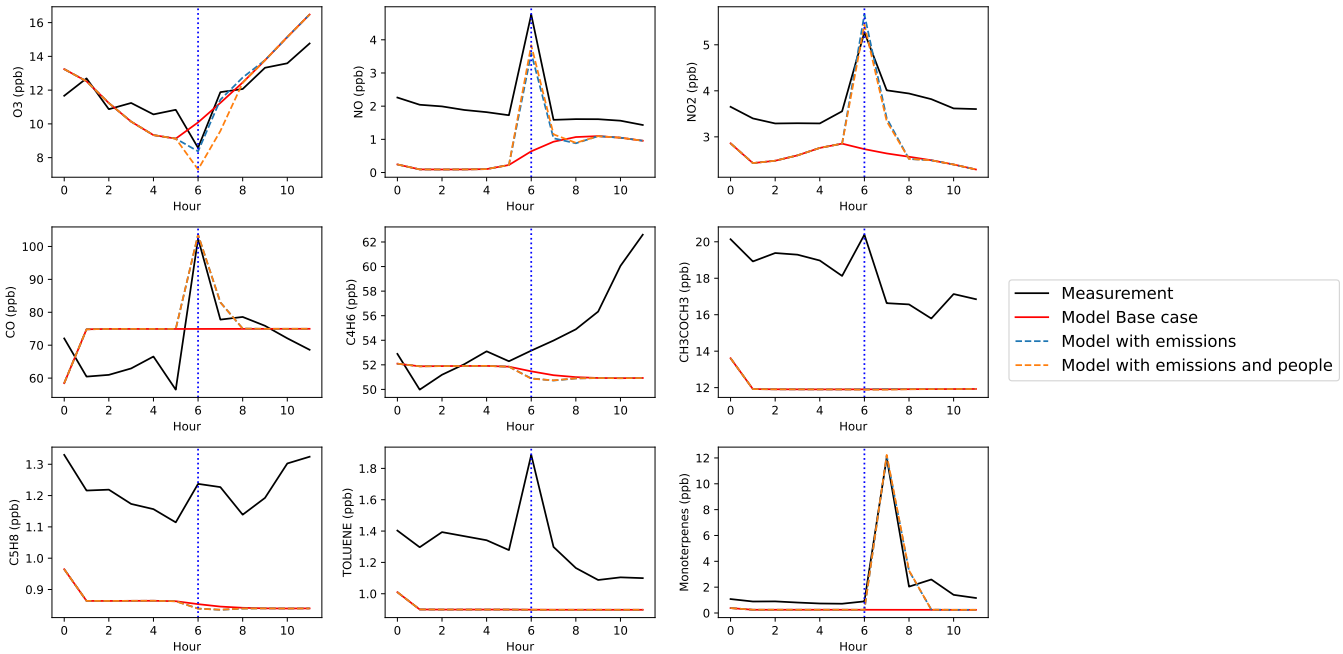
Indoor-outdoor exchange

- Indoor-outdoor exchange rate adjusted to match the diurnal profile of indoor O_3, NO_x, CO (excluding the activity periods): AER $= 5$ hr^{-1}.



Kitchen activities

- Emissions of NO_x, CO and monoterpenes (assumed to be limonene) tuned to match the observations during the morning activity periods.
- Model agreement with the observations improves for some species (O_3), but not of others (isoprene, acetone).



Summary & Future Work

- MBM-Flex is a flexible modelling framework designed to study air quality in indoor multi-room spaces.
- Reduced chemical mechanisms significantly cut down the computational cost of the model, with little impact on its accuracy.
- Cooking/cleaning related emissions can reproduce measured O_3, but the model tends to underestimate the observations of VOCs.
- Detailed activity logs are key for the interpretation of observations in indoor spaces.
- Future work will focus on improving the description of transport, indoor-outdoor exchange, and the representation of emissions.

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