Supplementary Material

Indoor Air Quality During Cooking and Cleaning: A Modelling Case Study in a Residential Kitchen Evaluated with Real-World Reference Instrument Measurements

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Table S1. Summary of structural and material characteristics of the simulated kitchen, including surface area, volume, material composition, lighting, and glass type.

Volume (m^3)	Surface Area (m^2)	Light Type	Glass Type	Paint (%)	Wood (%)	Metal (%)	Lino (%)	Plastic (%)	Glass (%)
24.52	56.40	Incand	glass_C	58.58	17.95	1.12	7.09	5.95	9.31

Table S2. Root Mean Square Error (RMSE) between modelled and observed indoor concentrations of O_3, NO, NO_2, and CO under different air change rates (ACRs), calculated during non-emission hours.

Species	ACR 5 h-1	ACR 6 h-1	ACR 7 h-1	ACR 8 h-1	ACR 9 h-1	ACR 10 h-1
O3	2.87	2.30	2.03	1.96	2.03	2.16
NO	2.08	2.08	2.07	2.07	2.07	2.06
NO2	0.80	0.78	0.76	0.75	0.74	0.74
CO	17.61	17.61	17.61	17.61	17.61	17.61

Table S2 summarises the sensitivity of model-measurement agreement to the assumed air change rate (ACR) during non-emission hours, quantified using RMSE for O_3, NO, NO_2 and CO. Among the four species, O_3 shows the strongest sensitivity to ACR, with RMSE decreasing from 2.87 at 5 h^{-1} to 2.03 at 7 h^{-1} and reaching a minimum of 1.96 at 8 h^{-1}, before increasing slightly again at higher ACR. This behaviour reflects the strong dependence of indoor O_3 on ventilation-driven exchange with outdoor air, while also indicating that O_3 should not be treated as a fully conservative indoor tracer because it is subject to surface deposition and chemical loss.

NO_2 shows a weaker but still systematic improvement with increasing ACR, with RMSE decreasing gradually from 0.80 at 5 h^{-1} to 0.74 at 9–10 h^{-1}. By contrast, NO shows very limited sensitivity to ACR, with RMSE varying only marginally between 2.08 and 2.06 across the tested range, while CO shows no sensitivity at all, with an

identical RMSE of 17.61 for all scenarios. These results indicate that the different species do not point to exactly the same optimum ACR, and that CO and NO provide limited discrimination between cases during the selected non-emission period.

Taken together, the results suggest that O_3 and, to a lesser extent, NO_2 favour intermediate-to-higher ACR values, whereas the overall multi-species comparison does not provide strong support for selecting the highest tested ACR. For this reason, an ACR of 7 h^{-1} was retained as a balanced choice across species, rather than selecting a value based on O_3 alone.

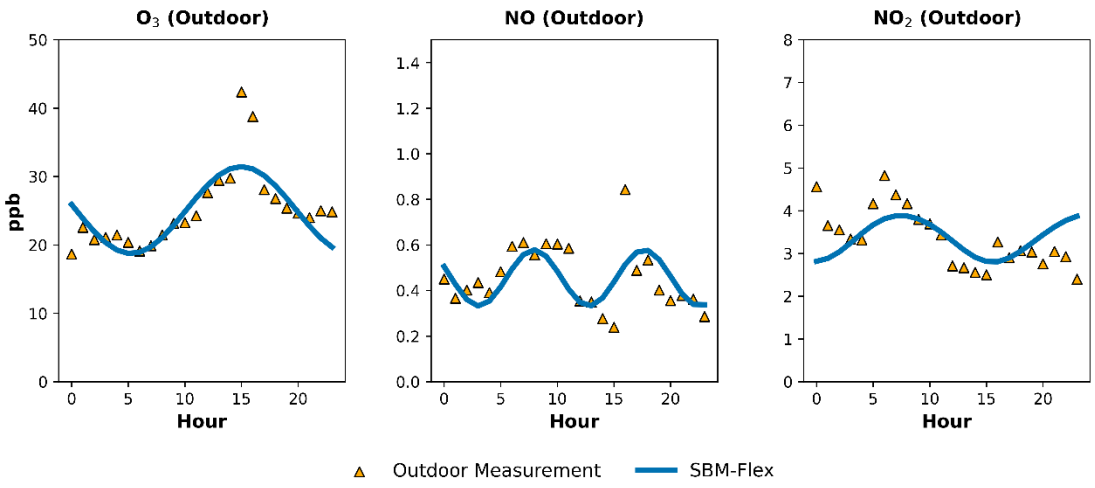

Figure S1. Diurnal cycles of outdoor O_3, NO, and NO_2 on 17 August derived from observed hourly averages and used as input boundary conditions in the indoor model.

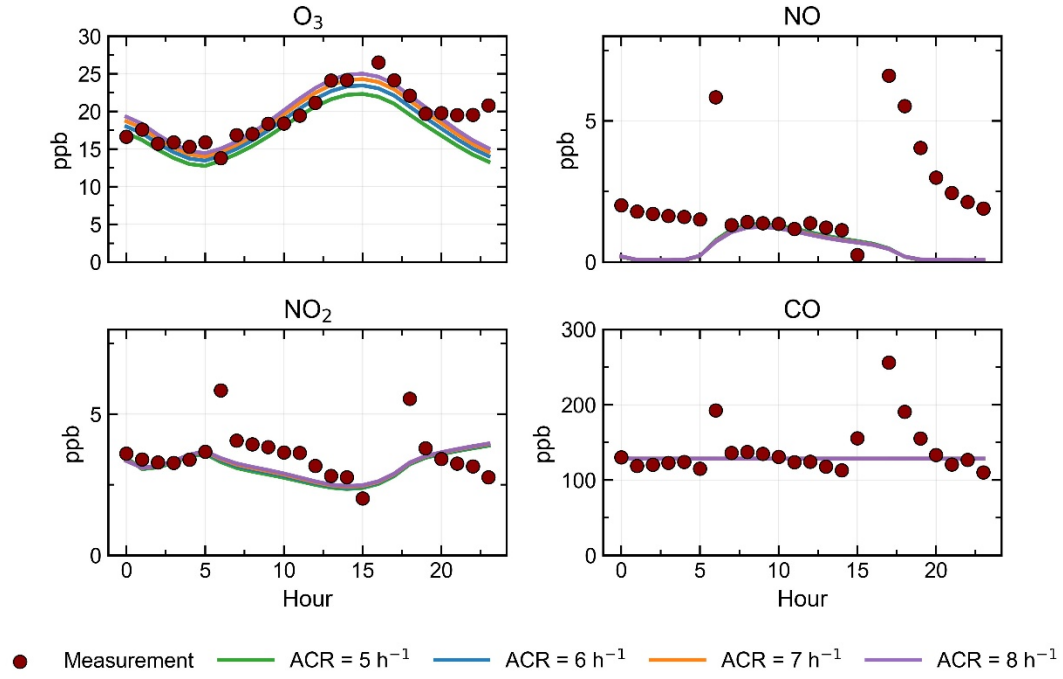

Figure S2. Optimisation of the air change rate (ACR) based on indoor diurnal profiles of gas-phase species primarily influenced by indoor–outdoor exchange (O_3, NO, NO_2 and CO). Periods associated with cooking and cleaning were excluded from the fitting. Measurements are shown as points, and model results for different assumed ACR values (5–8 h^{-1}) are shown as lines.

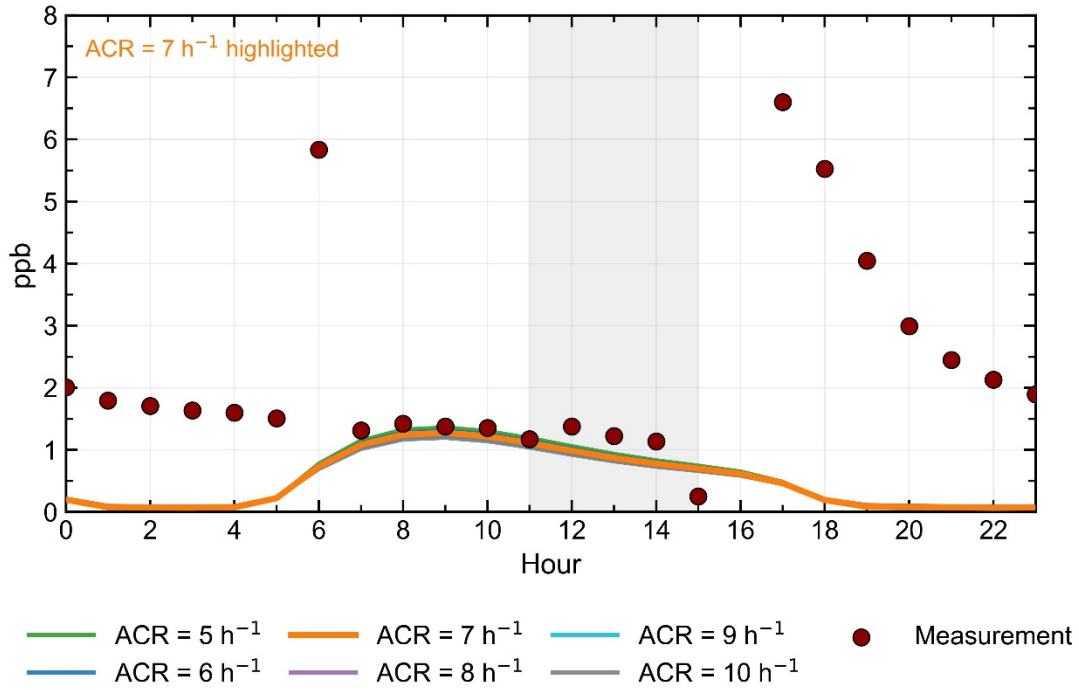

Figure S3 Comparison of measured and simulated NO concentrations under different assumed air change rates (ACR ranging 5–10 h^{-1}), with emphasis on the midday period.

This figure provides an additional diagnostic test of the ACR choice by showing how NO responds to increasing ventilation. Higher ACR values do not improve the reproduction of midday NO behaviour, supporting the retention of an ACR of 7 h^{-1} as a balanced choice across species.

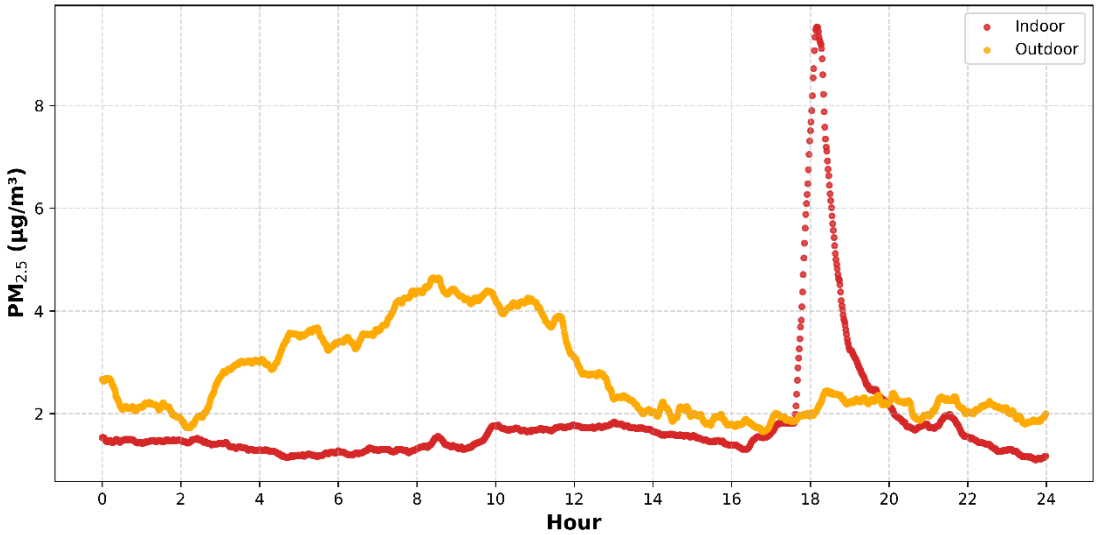

Figure S4. Minutely indoor (adjacent living room) and outdoor $PM_{2.5}$ concentrations measured on 17th August 2023.

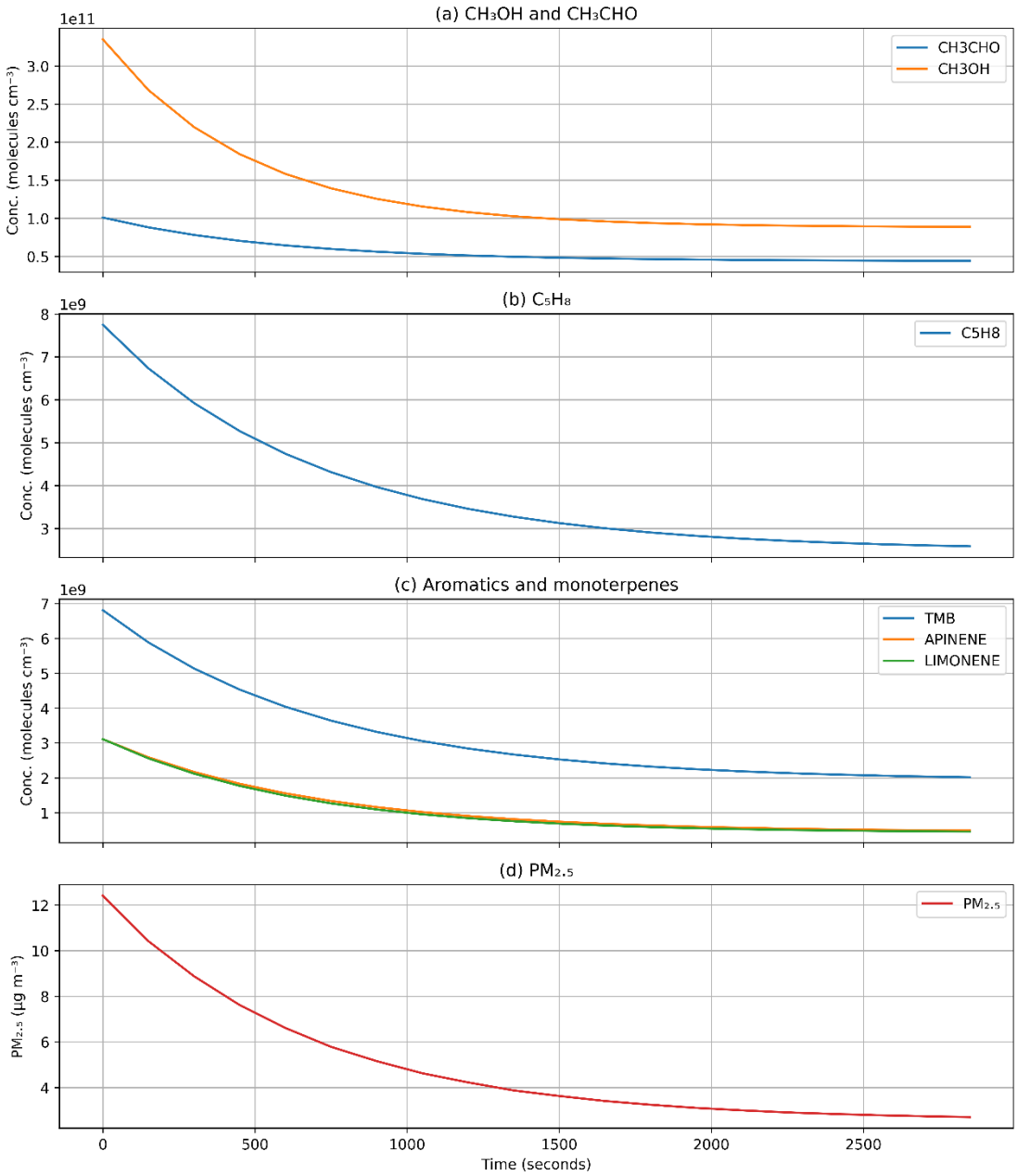

Figure S5. Early-time decline of reactive VOCs and $PM_{2.5}$ during the early simulation steps base case simulation.

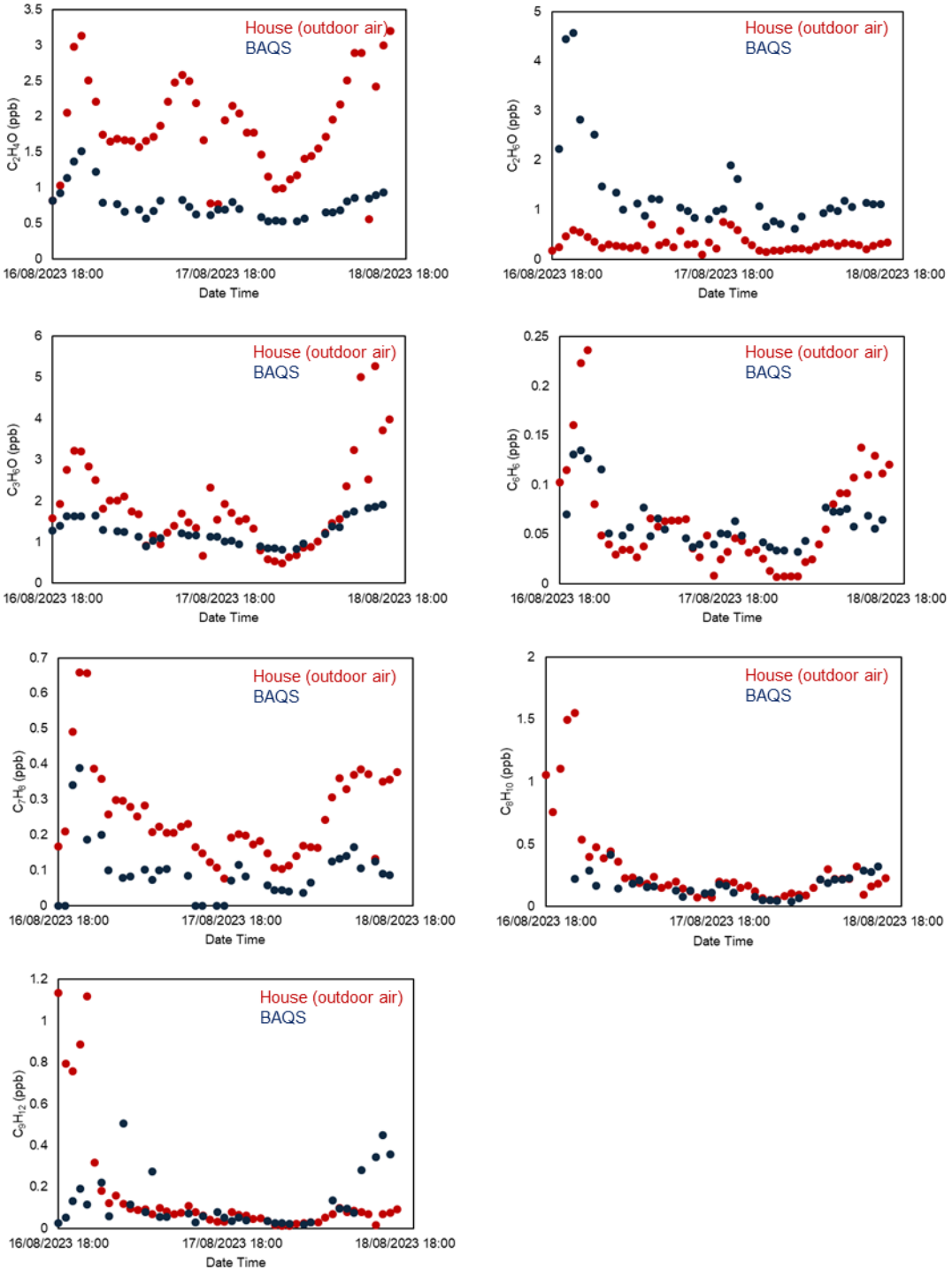

Figure S6. Comparison between outdoor VOC mixing ratios measured using PTR-ToF-MS at the experimental house and VOC mixing ratios measured using GC-MS at the Birmingham Air Quality Supersite (BAQS)

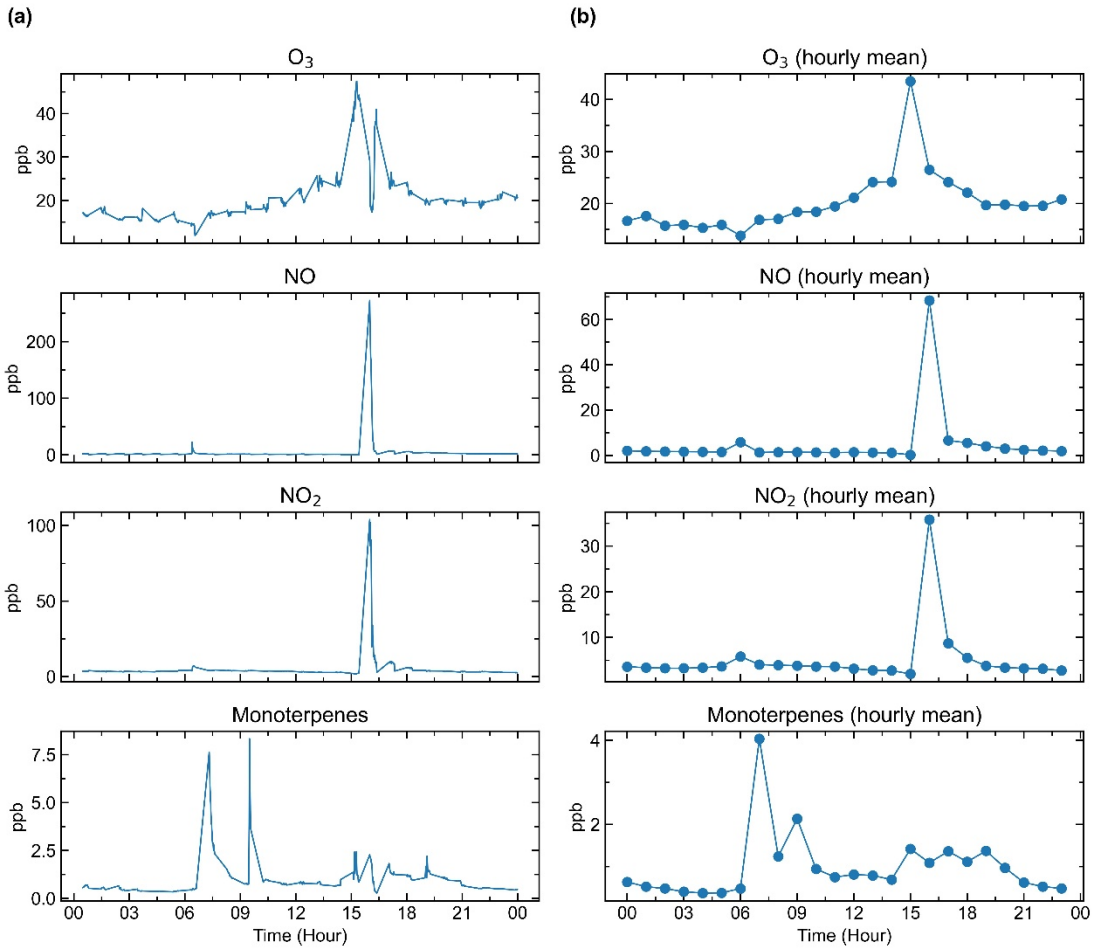

Figure S7. Illustration of the effect of hourly averaging on event signals. (a) High-time-resolution indoor measurements (native instrument resolution) for O_3, NO, NO_2 and monoterpenes, showing clear short-duration concentration enhancements associated with cooking and cleaning events. (b) The same data shown as hourly means for comparison with figures in the main text.

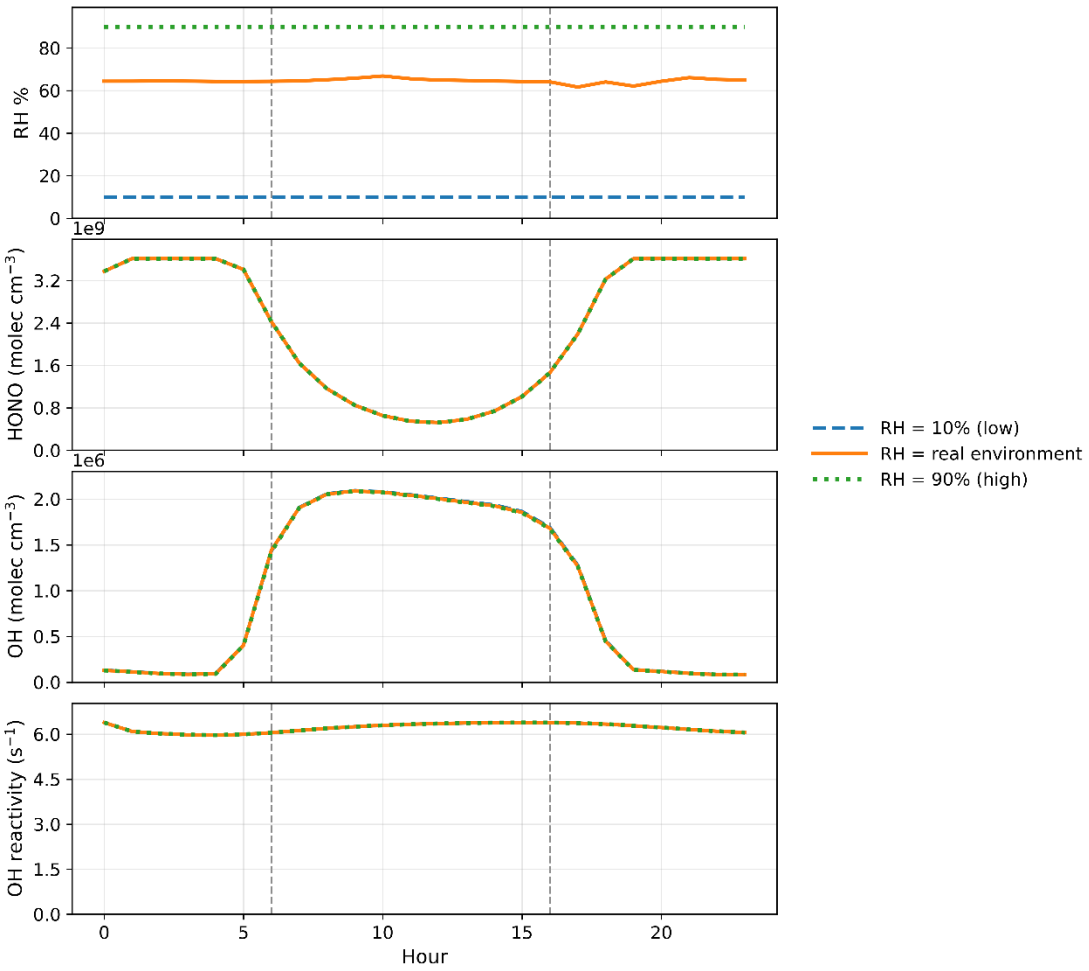

Figure S8. Sensitivity of simulated HONO, OH and total OH reactivity to relative humidity. The baseline simulation uses the observed indoor RH measured in the kitchen (~65%), while additional simulations with fixed RH values of 10% and 90% represent idealised sensitivity cases used to assess model behaviour.