# SAQN Awards End of Project Report

**Project Title:** Experimental Validation of Lagrangian Stochastic Methods targeting indoor air quality.

**Project Team**

| Name | Role (PI / Co-I) |
|---|---|
| Stefano Rolfo | PI |
| Terry Dillon | Co-I |

**Proposed activities (copy from your project proposal)**

During the SAQN scoping study “Exploring how sources, behaviour and mitigation strategies influence Indoor Air Quality: A Pilot Study”, initial CFD modelling was carried out, involving hydrodynamics and pollutant dispersion and simulations within the DOMestic Systems Technology InCubator (DOMESTIC) test house facility, originally hosted at the University of Chester. The dispersion of pollutants, resulting from cooking activities, was modelled using a scalar diffusion approach, where extra transport equations were included in the model to track the pollutant concentration within the domain. This approach has been proven suitable for modelling gas phase dispersion of $CO_2$, for instance, but when looking at particulate matter (PM) the comparison has been less favourable. This is a consequence of the very simplified approach used to model pollutant dispersion that does not consider several physical phenomena, as, for instance, the Brownian effects on the particle motion. The aim of this project is to use Lagrangian Stochastic Methods to track the particulate motion within the flow field and to perform this for several different pollutants resulting from different indoor activities. Further validation data is required to better characterise the pollutant sources, and this will be obtained from the relocated DOMESTIC facility at University of York.

The Work Packages for this project can be summarised as follows:

WP1:

- Numerical Modelling of particulate matter within the DOMESTIC test house – use of the Lagrangian Particle Tracking method with both Reynolds Averaged Navier Stokes (RANS) and Large Eddy Simulation (LES) turbulence modelling and comparison of the two approaches with each other and with experimental results.

WP2:

- Reinstallation and re-equipment of the DOMESTIC facility in York, followed by series of practical experiments investigating the impact of a range of kitchen-focused activities on indoor air quality.

WP3:

- Dissemination – promoting the applications of High-Performance Computing (HPC) techniques coupled with modelling amongst the air quality research community, and raising the profile of indoor air quality research amongst the HPC and Computational Fluid Dynamics (CFD) communities. Provision of experimental and simulation data to the STFC DAFNI platform.

**Please report on the activities completed in the project**

**WP1**- Numerical Modelling of particulate matter of a range of sizes within the DOMESTIC test house

As highlighted in the Chief Medical Officer for England's 2022 Annual Report, while outdoor air pollution is being successfully reduced, indoor air pollution remains a serious and under researched problem (Whitty et al., 2022). Approximately 4% of deaths worldwide are believed to be directly attributable to household air pollution, with a high proportion of these deaths being attributed to the inhalation of particulate matter with a diameter of less than 2.5 μm, known as $PM_{2.5}$ (WHO, 2022). While the exact mechanisms are still under investigation, research points towards the inflammatory effect generated by the embedding of these particles in the tissue of the respiratory system, causing and exacerbating morbidities such as ischaemic heart disease, stroke, respiratory infections, chronic obstructive pulmonary disease (COPD) and lung cancer (Thangavel, Park and Lee, 2022; WHO,2022). Within domestic settings, cooking has been identified as being a significant source of $PM_{2.5}$ (Chao and Cheng, 2002). A better understanding of the impact of cooking on indoor air quality is therefore required, and this is a research field in which numerical models can both complement and extend the capabilities of practical experimentation.

The current project builds on the SAQN scoping project "Exploring how sources, behaviour and mitigation strategies influence Indoor Air Quality: A Pilot Study" by Stevenson et al., (2021), and couples computational fluid dynamics (CFD) modelling with the Lagrangian Particle Tracking (LPT) approach detailed in Minier (2015), to model particulate matter dispersion within the DOMESTIC test house during cooking events. DOMESTIC is a controlled environment measuring 5.80 x 2.20 x 2.30 m and contains a full-scale kitchen/diner (equipped with an electric cooker) and a bathroom (see Figure 7 for a photograph of the interior layout). Full details of this test house, and the range of cooking experiments performed within it, are given below, under WP2.

*Figure 1*. Visualisation of particulate matter dispersion in DOMESTIC in the early stages of cooking.

As all cooking experiments were performed with the door between the kitchen and bathroom closed, only the kitchen portion of DOMESTIC was modelled. In the model, the walls of the test house were designated as being adiabatic, with the floor and ceiling having a temperature of 10 ℃ (from the experimental conditions). A heat source with a surface temperature of 180 ℃ was used for the frying pan, which was located on the back right ring of the cooker, as in the experiments (see Figure 1). Completely sealed conditions were assumed. A standard Eulerian single phase incompressible flow model was used, along with the Boussinesq approximation in the buoyancy term. The physical properties of the bulk phase (density, viscosity, specific heat and thermal conductivity) were set to the literature values of air at 11 ℃, the bulk room temperature.

LPT requires the tracking of each individual particle's trajectory, and thus is highly computationally intensive. For this reason, of the cooking experiments performed in DOMESTIC, the stir fry cooks were selected as being the most appropriate for modelling. These were of the shortest duration (12 minutes, after which the pan was sealed and removed from the test house) while still producing high local concentrations of particulate matter. The CFD solver used in this project was *Code_Saturne* (version 7.0), an open-source finite volume solver which is developed and maintained by EDF R&D (Archambeau, Méchitoua and Sakiz, 2004). As the finite volume method entails the division of the computational domain into multiple smaller volumes, or 'cells', in which the governing equations of fluid flow are solved, the number of these cells (the "mesh size") impacts the overall accuracy of the solution. For this reason, two different sizes of block-structured mesh were investigated – 41 and 171 million cells. This project also explored the relative performance of the RANS and LES turbulence modelling approaches in the context of these turbulent, poly-dispersed flows within small-scale domestic setting. The Elliptic-Blending Reynolds Stress Turbulence Model (EBRSM) was used as the example of a RANS approach, compared with the Dynamic Smagorinski and Wall-Adapting Local Eddy-Viscosity (WALE) models for the LES approach. Historically, the RANS approach has been more widely used due to its lower computational cost, but a high fidelity (LES) approach offers the potential for greater realism in such small-scale contexts (Blocken, 2018). A successful application was made for compute time on the Tier 1 supercomputer ARCHER2 via an EPSRC Access to HPC call, and all simulations were run here.

Figure 2 shows the simulated vs experimental results for air velocities within the test house. Experimental data was gathered using two Gill Instruments Windsonic ultrasonic 2D anemometers placed near the cooking source, which measured velocity in the U (positive x) and V (positive y) directions (for their location and alignments, see Figure 8). The experimental velocity range was extremely low, between a minimum of - 0.2 m $s^{-1}$ and a maximum of 0.15 m $s^{-1}$. This made it challenging to eradicate the effect of experimenter movement on the readings. The simulated velocities generally follow the trend of the experimental velocities (although with a smaller range) with the exception of the readings for anemometer 2 in the U direction, where all simulations strongly underpredicted the observed negative experimental velocities (see Figure 2, e and f). It is possible that this is attributable to the steam generated by the stir frying process, as the model did not incorporate a phase change. There was little difference between the performance of the three turbulence models, nor did refining the mesh to 171 million cells for the Dynamic Smagorinsky and WALE cases appreciably alter the results. The reproducibility of these results across different simulations and turbulence models suggests that the case itself is reliably constructed, but may require additional parameters to align it more closely with the experimental conditions. It is also important to note that the anemometers used were clustered in the vicinity of the source, and were 2D, meaning that the velocities along the z-axis (vertically upward) could not be captured (Gill Instruments, 2021). The use of a greater number of 3D anemometers, distributed across the domain, would be required to fully characterise the fluid flow in the bulk of the container.

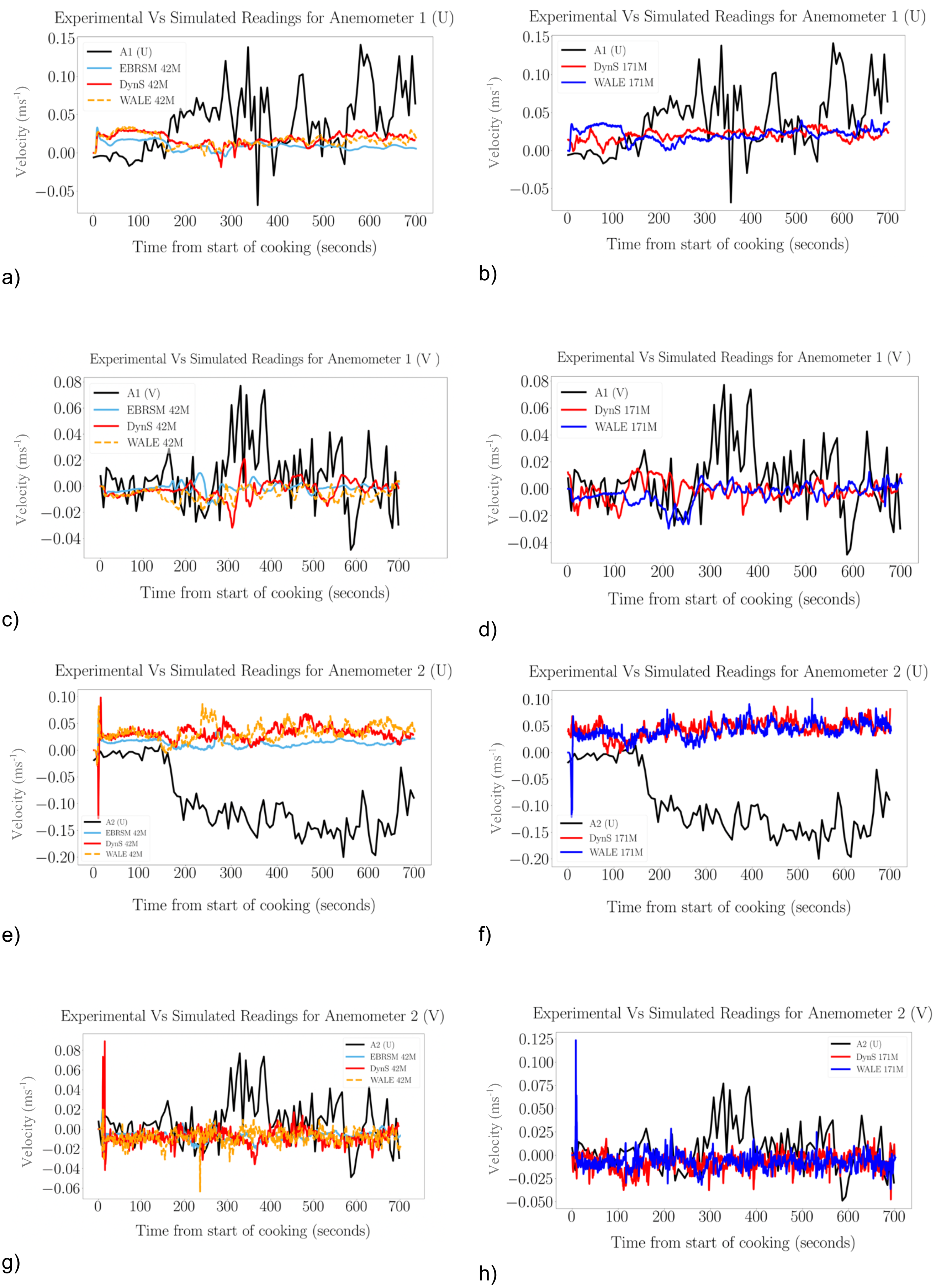
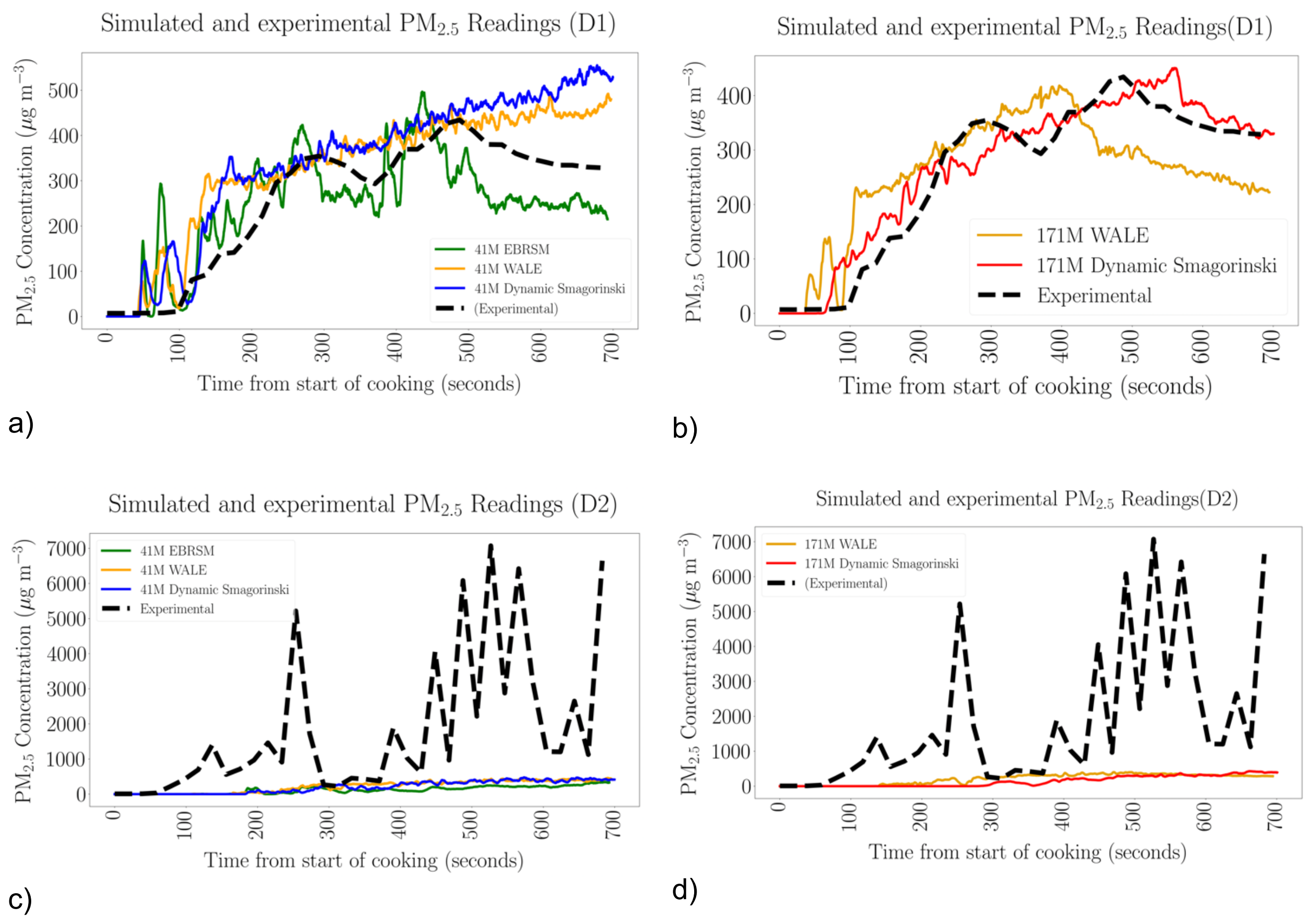



*Figure 2*. Comparison of experimental (A1 and A2) and simulated velocities for anemometers 1 (A1) and 2 (A2) for tofu stir fry experiments.

To simulate the dispersion of $PM_{2.5}$ during cooking, particles were injected into the computational domain immediately above the location of the pan, at a rate of 1.6 mg min$^{-1}$ (from the experimental readings and Shrubsole et.al., (2012)). Particle diameter was assumed to be 2.5 μm (with a variance of 0.7 μm) and particles were assumed to be of homogenous composition, with a density of 1.5 g cm$^{-3}$ (Shi et.al., 2015). Simulations generally compared well with the spatial experimental data generated from low cost NuWave sensors (for details on these sensors and their location see below in WP2). Here the LES approach considerably outperformed the RANS EBRSM approach, with the 41 million cell mesh WALE and Dynamic Smagorinski models both giving good predictions at sensor points D1,3,4, and 6, while the 42 million EBRSM model is less well fitted to the experimental data at these points (see Figure 3). The overall best fit to the experimental results was given by the 171 million cell mesh Dynamic Smagorinski model, indicating that, as expected, high resolution techniques offer the most promising avenue of investigation. All models underpredicted concentrations at D2, the sensor in close proximity to the cooking source. Again, this is likely to be due to the absence of steam and experimenter movement from the model – note the alternations between peaks as high as 7000 μg m$^{-3}$ and troughs of under 600 μg m$^{-3}$ seen in this experimental data at this sensor (Figure 3 (c) and (d)) which suggest that the sensor is being subjected to intermittent gusts of particle-laden air. All LES simulations underpredicted the concentrations of $PM_{2.5}$ at D5, the table-height sensor (Figure 3, (i) and (j), with the 41M WALE and Dynamic Smagorinski also showing a short but intense peak in concentration early on in the simulations, not seen in the experimental results. This peak is absent in the 171M Dynamic Smagorinski simulation, indicating that this may be an artifact generated by the coarser mesh.



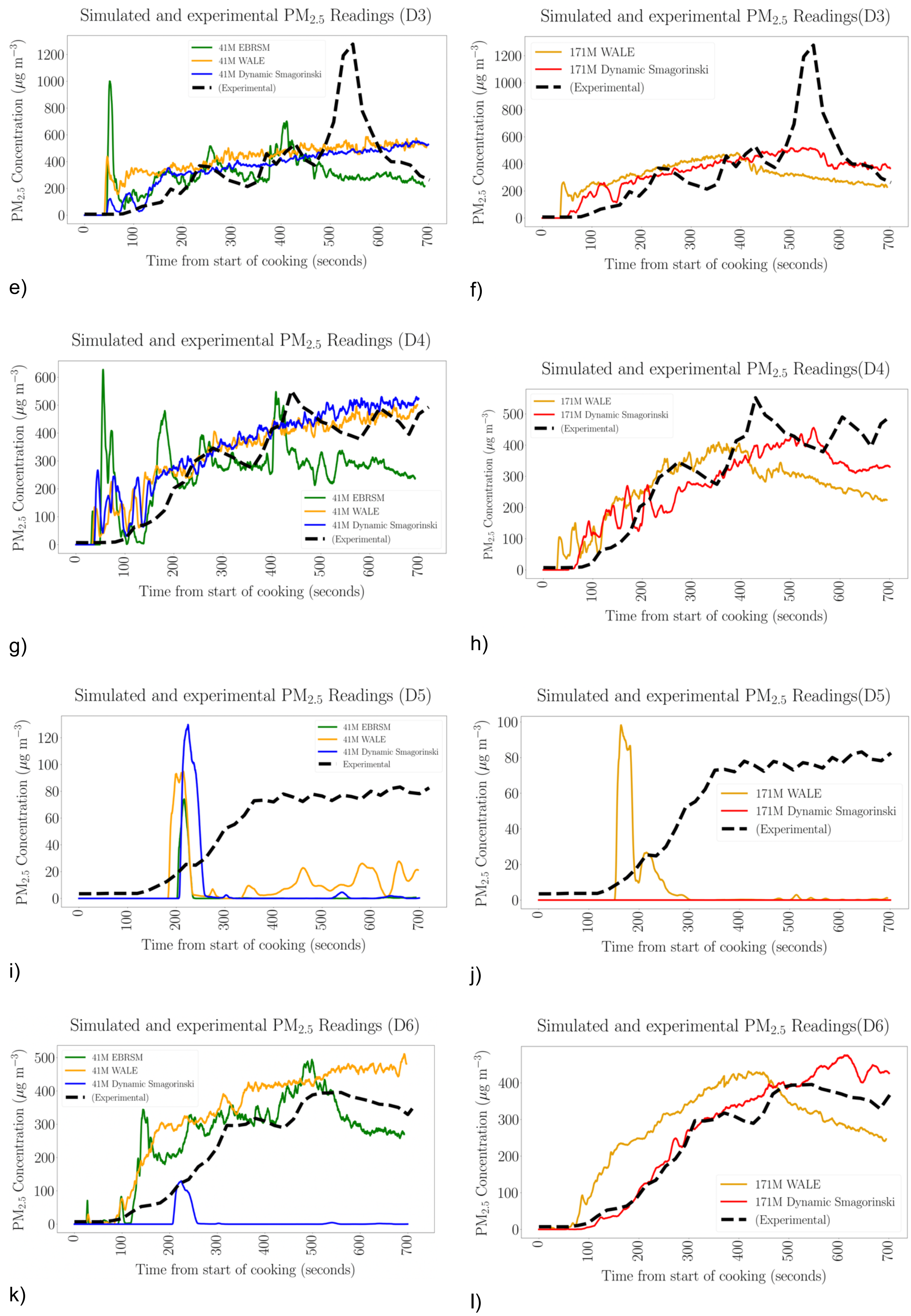



*Figure 3*. Comparison of mean experimental and simulated readings for $PM_{2.5}$ (tofu stir fry).

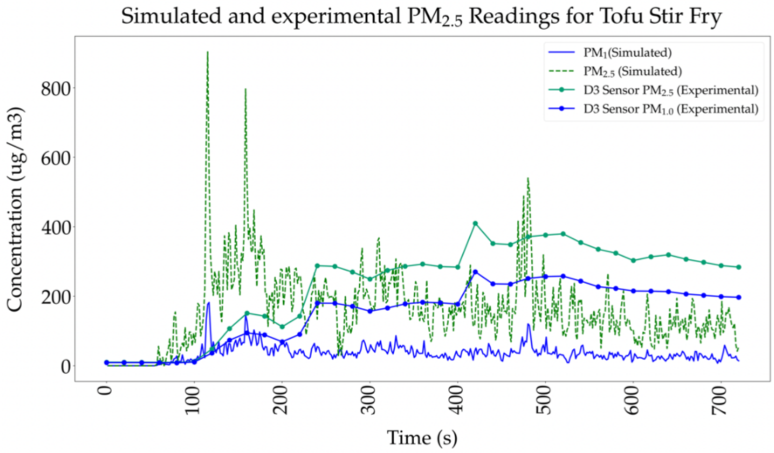
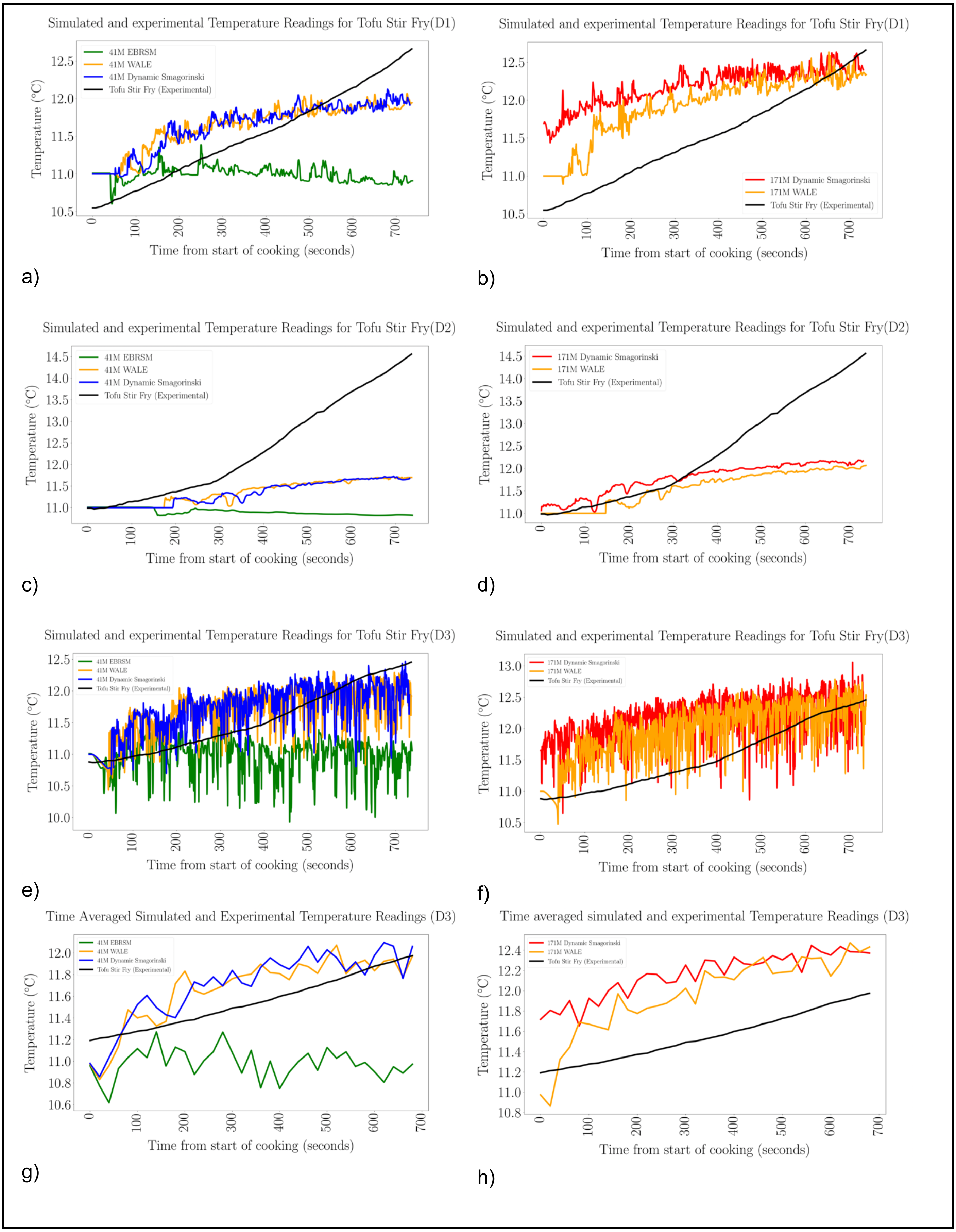



*Figure 4.* Comparison of simulated (using the EBRSM turbulence model) and experimental readings for $PM_{2.5}$ and $PM_1$ at the D3 sensor, using a single, preliminary cook of tofu stir fry.

Investigations were also made as to the feasibility of representing multiple different particle classes within the computational model, in order to be able to more precisely differentiate the distribution of $PM_{2.5}$ as a whole from $PM_1$, $PM_{0.5}$, etc. Test simulations comparing $PM_{2.5}$ and $PM_1$ were fairly successful, although with $PM_1$ generally underestimated (see Figure 4 for an example of this). For the current project it was deemed most appropriate to focus on the simulation of $PM_{2.5}$ only, with deeper investigation into the inclusion of other size demographics of particles being identified as an important subject for future research.

The simulated temperatures from the LES simulations showed some agreement with the experimental results for D1, 3 and 4 (see Figure 5).The noticeable noise in some of the simulated readings (see, for example, Figure 5 (e) and (f), are primarily due to the difference in measurement frequency between the simulations (0.04 seconds for the 42 million cell simulations, 0.002 seconds for the 171 million cell simulations) and the NuWave sensors (every 20 seconds). Averaging the simulation readings over a 20 second period removes the bulk of these oscillations, particularly for the 171M Dynamic Smagorinski and WALE cases (figure 5 (g) and (h)). All models underpredicted the rise in temperature seen at D2 (Figure 5 (c) and (d)), nor did they match the gradient of the temperature rise seen at D5 (Figure 5 (k) and (l).The requirement that the bulk fluid be initialised at a given temperature means that regions where the bulk temperature is below this (such as at D5, which was essentially at floor temperature) the model does not immediately reflect this. This effect is also seen at D6, where the EBRSM simulation begins and remains at 11 ℃. The LES simulations performed better here, but still underestimated the gradient of the temperature increase. All simulations also showed small peaks or troughs (+/- 0.2 ℃) not seen in the experimental temperature readings (Figure 5 (k) and (l). These artifacts have been identified as subjects for further investigation.



Simulated and experimental Temperature Readings for Tofu Stir Fry(D1)
41M EBRSM
41M WALE
41M Dynamic Smagorinski
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
a)
Simulated and experimental Temperature Readings for Tofu Stir Fry(D1)
171M Dynamic Smagorinski
171M WALE
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
b)
Simulated and experimental Temperature Readings for Tofu Stir Fry(D2)
41M EBRSM
41M WALE
41M Dynamic Smagorinski
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
c)
Simulated and experimental Temperature Readings for Tofu Stir Fry(D2)
171M Dynamic Smagorinski
171M WALE
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
d)
Simulated and experimental Temperature Readings for Tofu Stir Fry(D3)
41M EBRSM
41M WALE
41M Dynamic Smagorinski
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
e)
Simulated and experimental Temperature Readings for Tofu Stir Fry(D3)
171M Dynamic Smagorinski
171M WALE
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
f)
Time Averaged Simulated and Experimental Temperature Readings (D3)
41M EBRSM
41M WALE
41M Dynamic Smagorinski
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
g)
Time averaged simulated and experimental Temperature Readings (D3)
171M Dynamic Smagorinski
171M WALE
Tofu Stir Fry (Experimental)
Temperature (°C)
Time from start of cooking (seconds)
h)

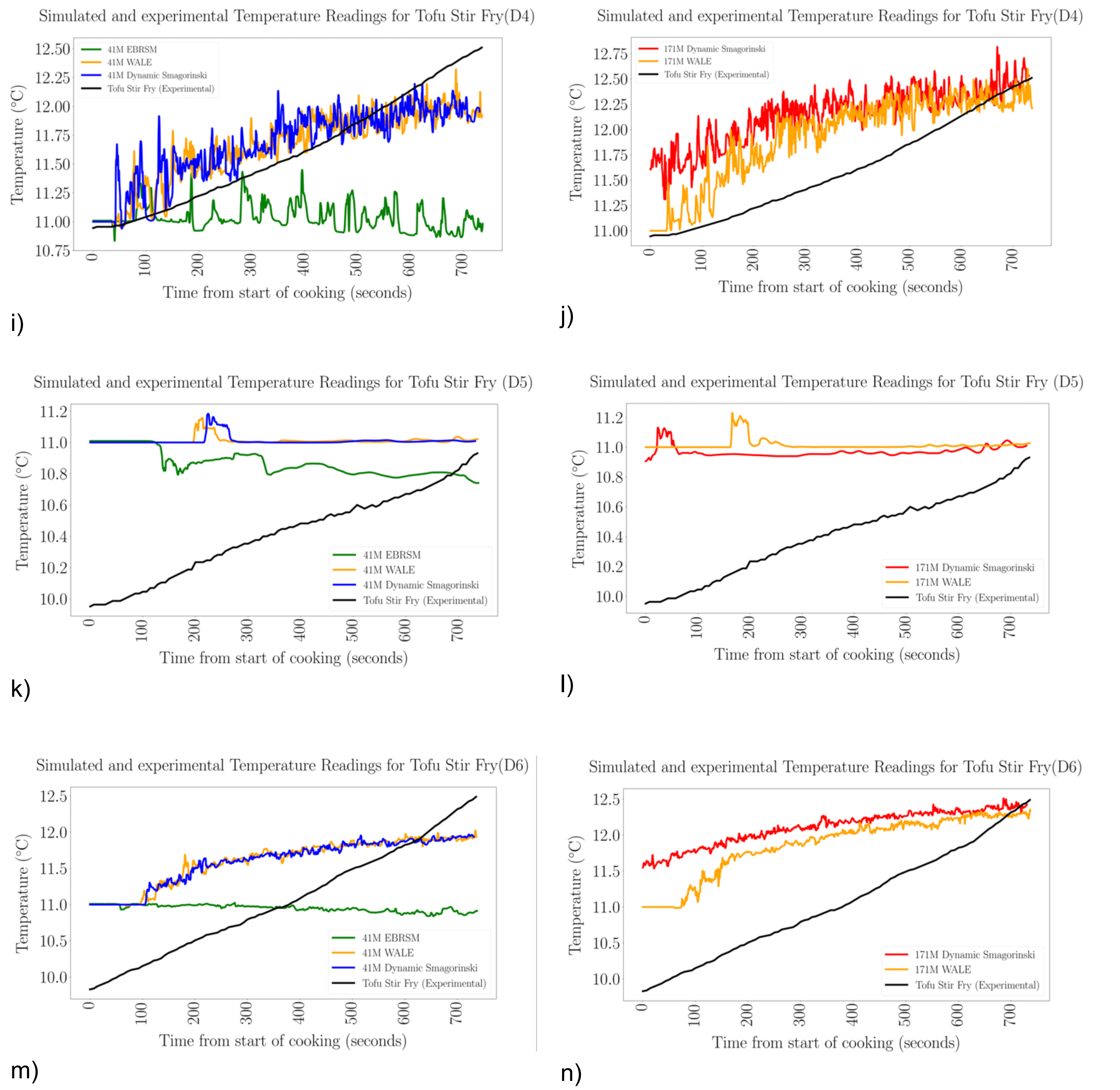



*Figure 5*. Comparison of mean experimental and simulated readings for temperature (tofu stir fry).

This project demonstrated successfully the superior performance of the LPT method to the scalar diffusion model used in the previous scoping study. As expected, the high-fidelity approach, using LES and a fine mesh, gave the best overall results. This illustrates the critical contribution that High Performance Computing (HPC) can make to the better understanding of air quality, and indicates how these could be applied in the wider context of Health and Environment. Elements of the simulation approach that remain to be improved include the factoring in of steam and experimenter movement, and the elimination of unfeasible artifacts within the temperature field.

**WP2** – practical experimentation in DOMESTIC

The DOMESTIC test house installation was successfully relocated from a site at the Thornton Campus at the University of Chester to the University of York in March 2022. The reinstallation timeline was unavoidably elongated due to administrative requirements, with the test house being fully equipped and functional by November 2022. As a result of this, it was necessary to slightly narrow the focus of the practical experimentation to concentrate on full-recipe cooking, in sealed conditions.

DOMESTIC consists of two converted shipping crates, each measuring 5.80 x 2.20 x 2.30 m (see Figure 6). The first is the test house itself, which contains a full-scale kitchen/diner (equipped with an electric cooker) and a bathroom (see figure 7). This can be ventilated, using a window or extractor fans, but can also be fully airtight if required. The second is the plant room, into which sampling lines from the test house are ducted. The plant room was equipped with $NO_2$ $NO_x$ $O_3$ and $SO_2$ analytics, along with a SYFT selected ion flow tube mass spectrometer. A low-cost QUANTAQ MODULAIR-PM sensor was placed on the exterior of the test house, and an identical unit was placed within the test house, for indoor-outdoor comparisons of PM concentrations (QuantAQ, 2021). The test house was also equipped with six low-cost NuWave AirSentric WB55 Wireless Indoor Air Quality Monitors. These sensors measure $CO_2$, $PM_1$, $PM_{2.5}$, $PM_4$, $PM_{10}$, temperature and humidity (Nuwave, 2022). Two Gill Instruments Windsonic ultrasonic 2D anemometers were placed in the vicinity of the cooker (for locations of all sensors and anemometers see figure 8).

*Figure 6*. Exterior of DOMESTIC on site at the University of York.


*Figure 7*. Interior of the DOMESTIC test house.

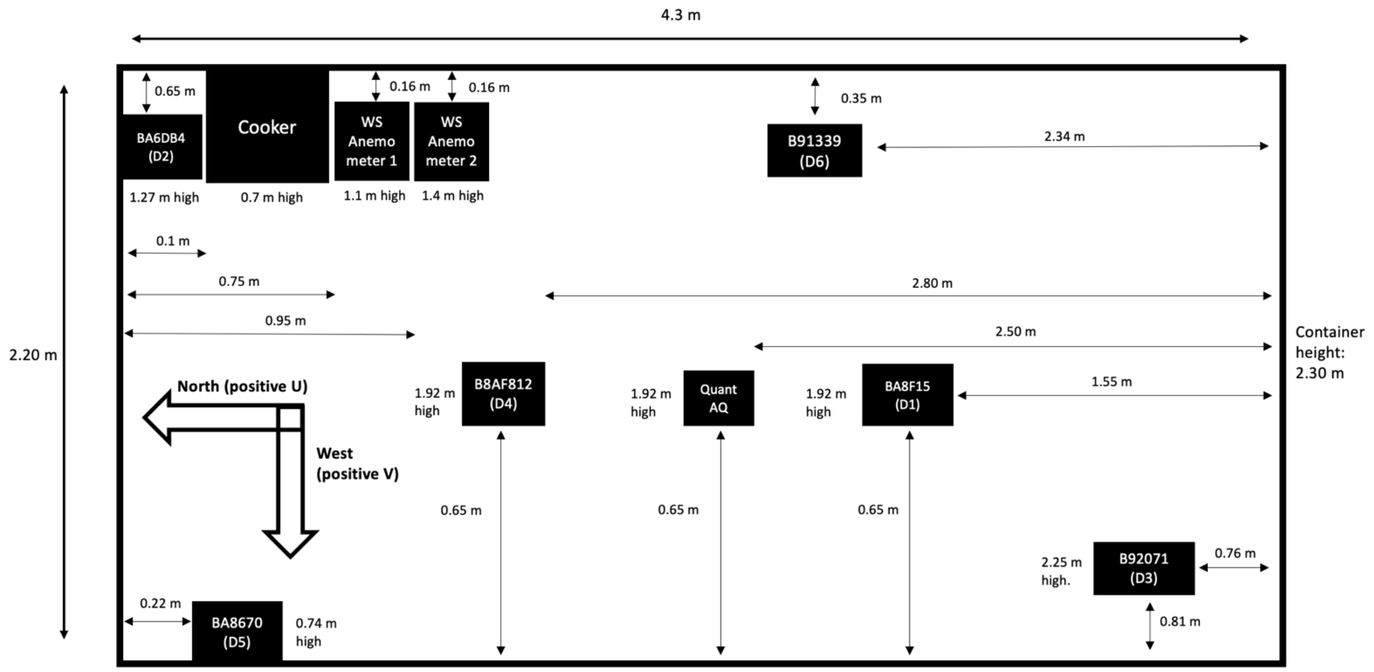



*Figure 8.* Locations of the Nuwave (D1-6) and QuantAQ sensors, and anemometers within the DOMESTIC test house (not to scale).

Three types of dishes were used for the cooking experiments: stir-fry, curry and chilli. In each case a meat and vegetarian version were compared - chicken stir fry vs tofu stir fry, chicken curry vs paneer curry, and beef chilli vs red bean chilli. Recipes were kept identical excepting the meat substitution. A minimum of three repeats were performed for each recipe, with the test house being allowed to return to baseline PM concentrations (around 4 µg $m^{-3}$ for $PM_{2.5}$) in between each cooking session. Figures 9-11 show the mean spatial $PM_{2.5}$ concentrations during these cooks. As the cooking duration for the various dishes varied (12, 21 and 26 minutes for the stir fry, curry and chilli respectively), and the total duration of experimenter time spent in the test house also varied, the approximate start and end time of each cooking procedure is indicated on the graphs. The spatial $PM_{2.5}$ concentrations were as expected, with the highest concentrations seen at the sensor nearest the cooker (D2) and the lowest at the table-height D5 sensor, which consistently gave readings that were a minimum of 10 times less than those at D2. In general, the trend was that the meat-based dishes caused slightly greater spatial elevations of $PM_{2.5}$ – this was as expected, as meats are known to be a strong source of $PM_{2.5}$ due to their fat content (Gysel et al., 2018). However, certain sensors registered higher average $PM_{2.5}$ concentrations for the vegetarian substitutes – see the QuantAQ readings for the stir fry (Figure 9) and the NuWave D3 readings for the curry (figure 10). This raises the issue of variability within these and similar cooking studies. Despite rigorous standardisation of the experimental protocol there was considerable variability in the readings between each cook. Figure 12 shows the QuantAQ and NuWave D3 sensor readings for all three runs for the stir fry and curry experiments, illustrating how in each case the average results are affected by a single run with readings that do not follow the broader trend. In the case of the NuWave D3 readings for the paneer curry, the maximum $PM_{2.5}$ concentration peak is found at 3000 µg $m^{-3}$ for run 2, and at around 400 µg $m^{-3}$ for runs 1 and 3. It is uncertain whether elements of the protocol, sensor performance, or other factors such as temperature conditions within the test house could be the cause – more extensive experimentation would be required to determine this. One noticeable point is that, while $PM_{2.5}$ concentrations almost immediately increase following the start of cooking for the stir fry and curry, concentrations during the chilli cooks only increase a few minutes before the end of cooking. This is likely to be due to the nature of the recipe, and indicates the importance of the investigation of a range of different dishes in order to properly comprehend their effect on the local environment.

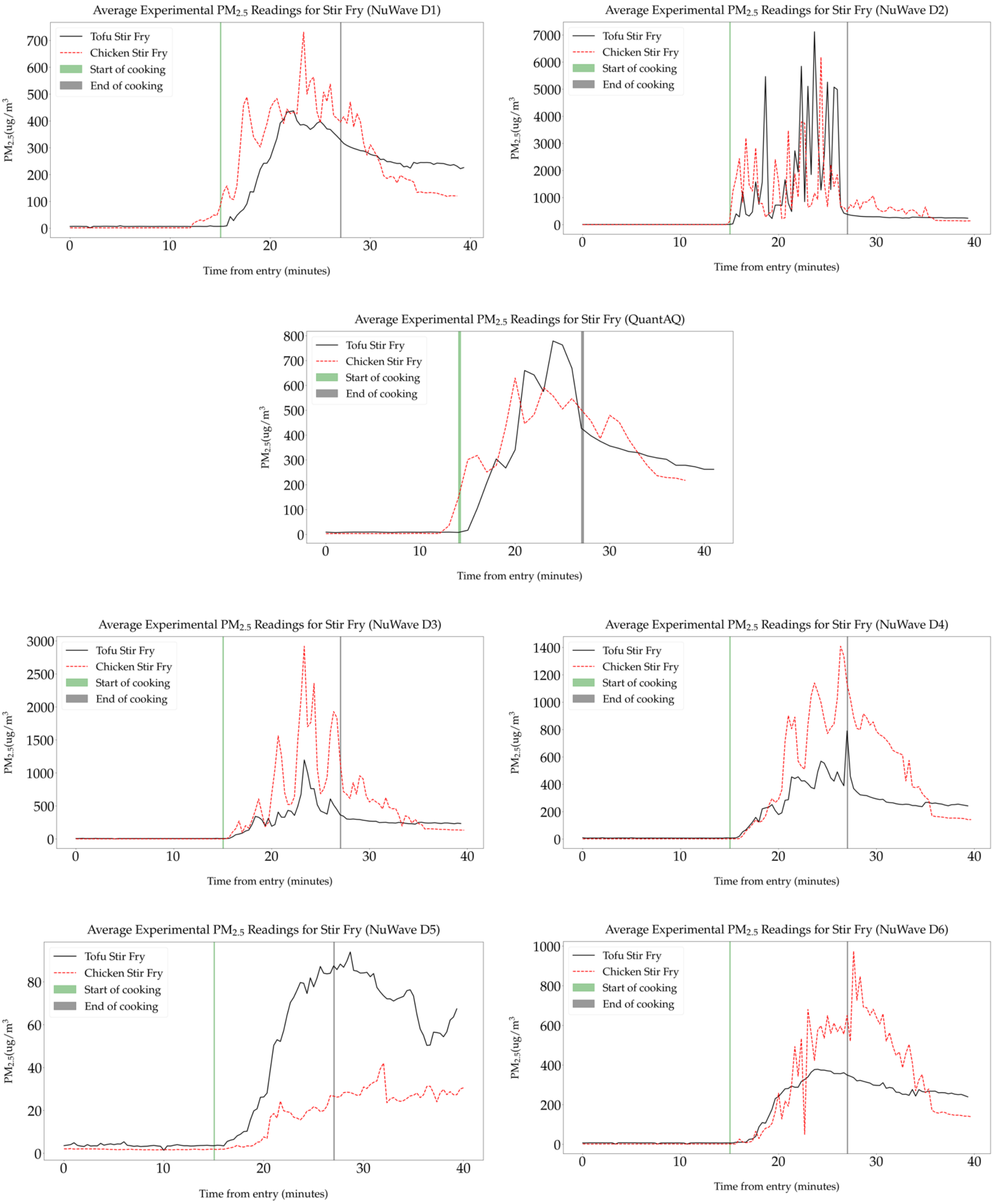



*Figure 9*. Comparison of average spatial PM$_{2.5}$ concentrations for vegetarian and chicken stir fry (NuWave and QuantAQ sensors).

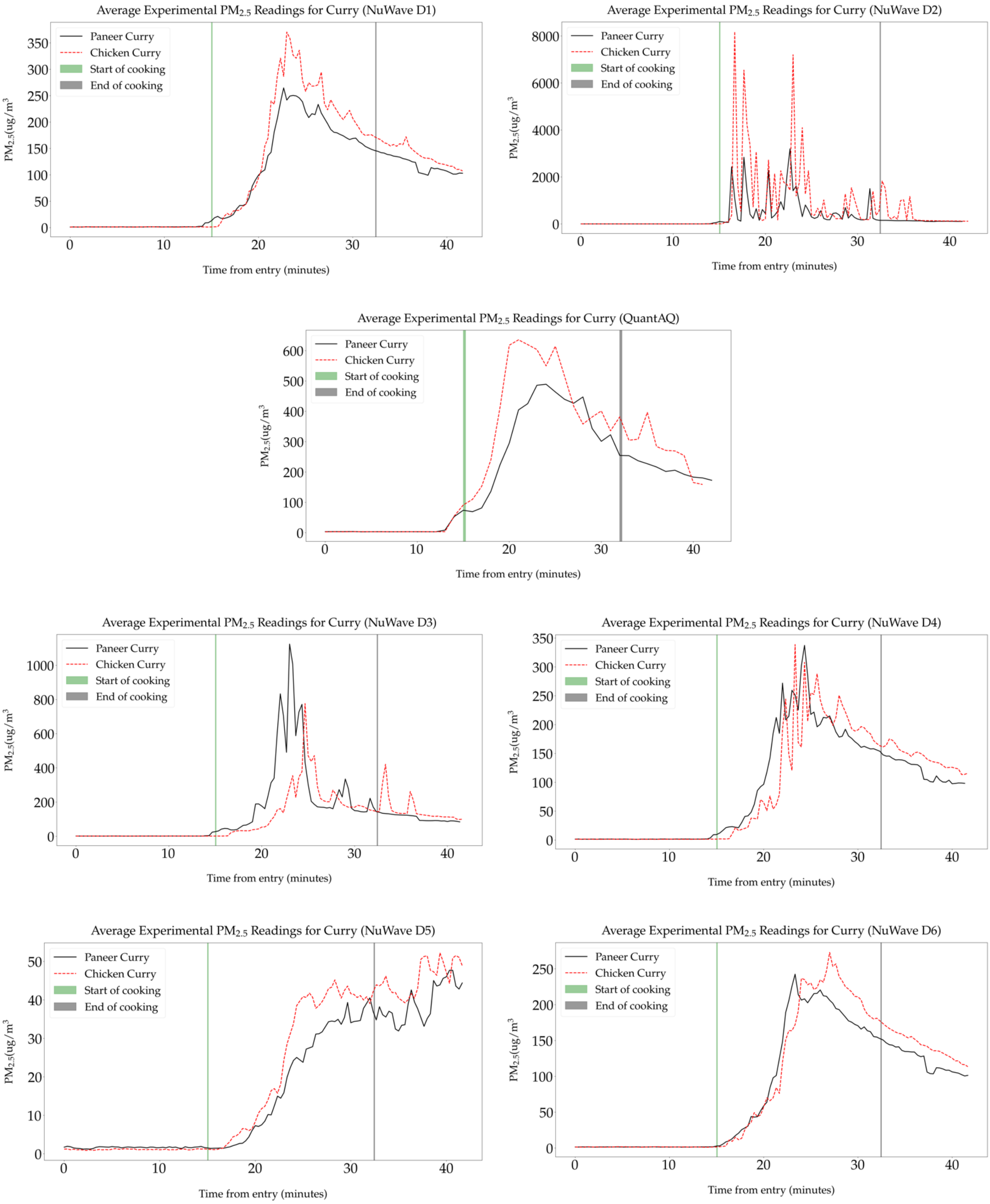



*Figure 10.* Comparison of average spatial $PM_{2.5}$ concentrations for vegetarian and chicken curry (NuWave and QuantAQ sensors).

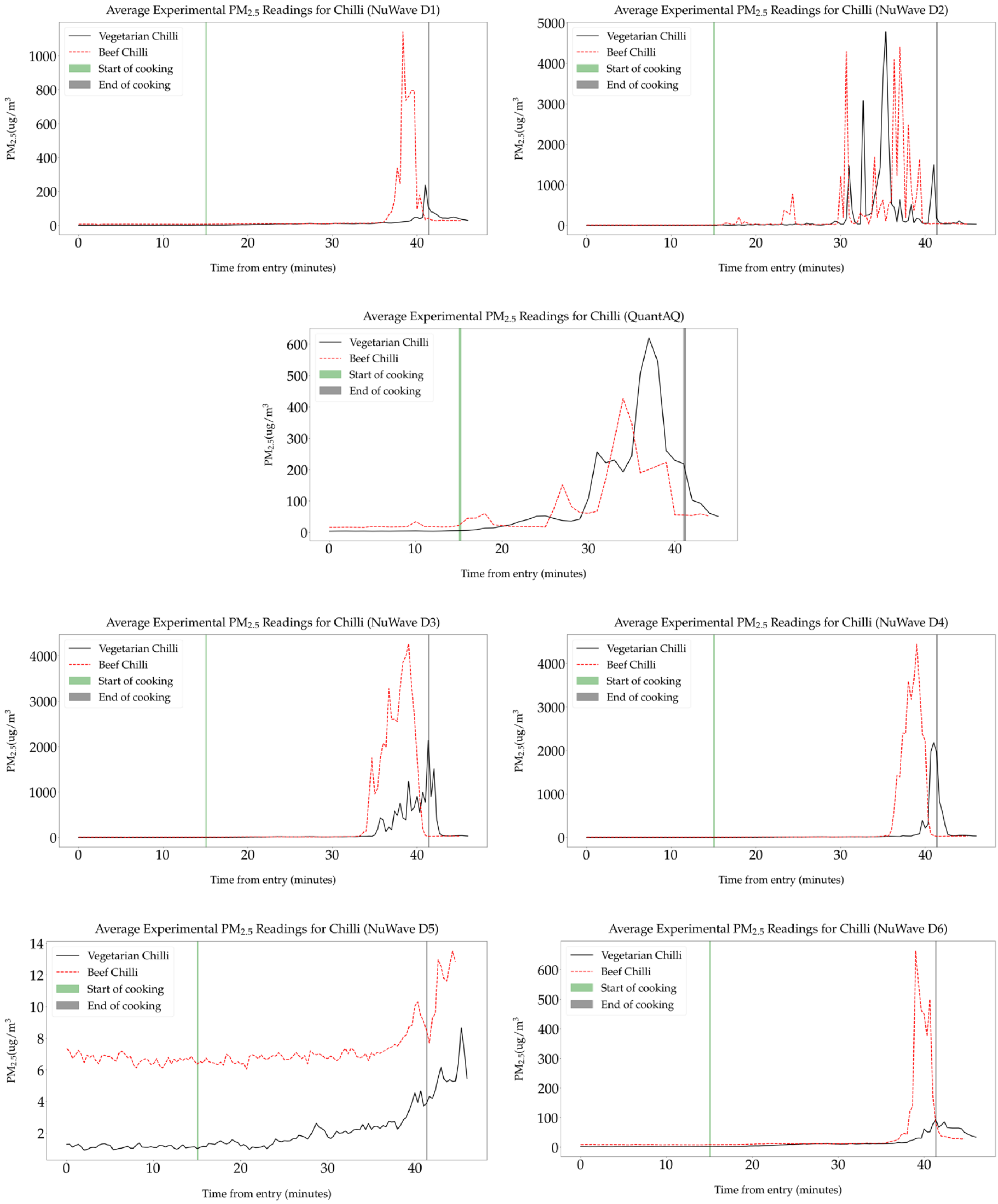



*Figure 11.* Comparison of average spatial $PM_{2.5}$ concentrations for vegetarian and beef chilli (NuWave and QuantAQ sensors).

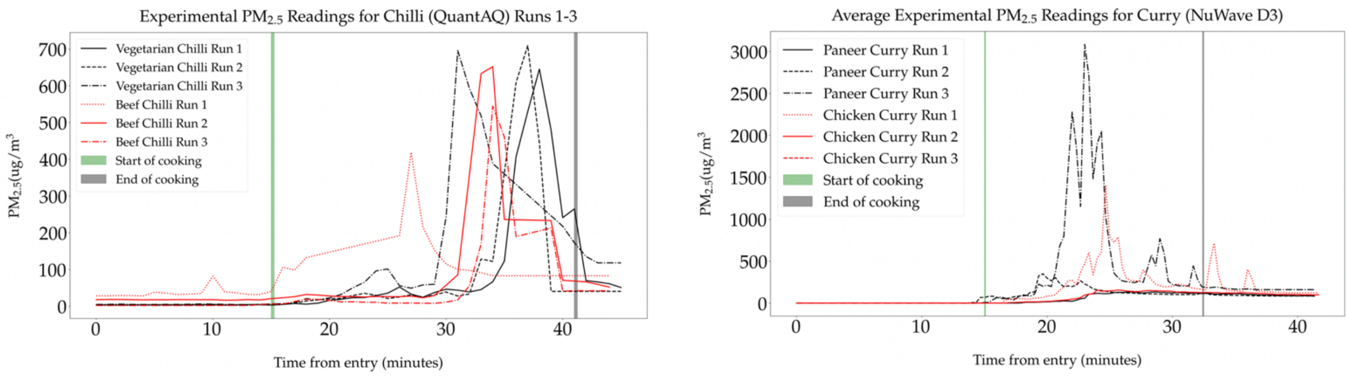



*Figure 12.* Examples of the variations in sensor readings between individual cooking experiments.

**WP3** – dissemination

Two conference contributions on this topic have been accepted, a presentation for the 2023 Parallel Computational Fluid Dynamics International Conference (ParCFD) and a poster presentation and paper for the 2023 ERCOFTAC symposium on Engineering, Turbulence, Modelling and Measurements (ETMM14). For a full list of dissemination activities, see below under ‘outputs and impacts’. The team are also currently in the process of collating and uploading the numerical and experimental databases generated by this project to the STFC Data and Analytics Facility for National Infrastructure.

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**What are the next steps for this research? Will you be applying for further funding? What will you need to continue researching this topic?**

Potential new funding opportunities are being evaluated to include modelling activities related to air quality as part of the digital research infrastructure (DRI). These activities are led by the scientific computing department and are funded by UKRI to promote cross disciplinary and cross council research.

**Please outline the role of STFC in this project**

All numerical modelling was undertaken by a team within the Engineering and Environment Group of STFC's Scientific Computing Department (SCD). The STFC SCD Year in Industry student attached to the project also assisted in the practical experimentation process.

**Please list a brief list of all outputs and impacts below. These may include papers, articles or blogs, presentations at events or conferences, meetings about future plans for the research. Please include links wherever possible**

- Successful application for the EPSRC Access to HPC, enabling the project to make use of the UK's Tier 1 supercomputer.
- Details of the project presented during the Manchester *Code_Saturne* Developers meeting, November 2022.
- Project poster displayed at Computing Insight UK, December 2022 (https://www.scd.stfc.ac.uk/Pages/CIUK-2022-Poster-Competition.aspx)
- Future research plans discussed as part of the UK Turbulence Consortium Annual Meeting, Imperial College London, 2023.
- Project featured as part of the IMPacts of Cooking and Cleaning on indoor Air quality: towards healthy BuiLdings for the futurE (IMPeCCABLE) end of project workshop, University of York, 2023 (https://impeccable.york.ac.uk/workshops).

**Were there any unexpected outcomes as part of the project?**

During the project, it was found that there were certain elements in the structuring of the Lagrangian Particle Tracking module in *Code_Saturne* which presented issues when combining it with the LES approach. The Computational Engineering Group of the Scientific Computing Department at STFC has a long-standing connection to the EDF R&D team, and it is now intended that data from this project will be used to enhance the performance of the module in this area. This will widen the scope of the module for use in future high resolution air quality simulation projects.

**What are your plans to share the outcomes of this research with others? (Give details of any future meetings, conferences, papers or other dissemination planned)**

- Two conference contributions on this topic have been accepted, a presentation for the 2023 Parallel Computational Fluid Dynamics International Conference (ParCFD) and a poster presentation and paper for the 2023 ERCOFTAC symposium on Engineering, Turbulence, Modelling and Measurements (ETMM14).
- A poster covering this research will be displayed at an STFC networking event surrounding the July 2023 Birmingham Clean Air Conference.
- Videos describing the project's structure and results will be shown during the STFC Daresbury Laboratory 2023 Open Day event.
- The project will be featured in a presentation at the *Code_Saturne* user meeting at EDF Lab Paris-Saclay in October 2023.

**Project Impact: What is the most significant output/impact from this project?**

This project has shown to STFC senior management the potential of current modelling and simulation capabilities within STFC to support air quality research. These activities are naturally multi-disciplinary and cross council and are now being considered to be part of the next wave of activities for the Digital Research Infrastructure funding from UKRI. This funding can underpin a wealth of opportunities for the air quality community in the UK.
A second important output is that the project has highlighted some deficiencies in the LPT module inside Code_Saturne that can now be addressed together with the Code_Saturne development team. Some good validation data have been produced and this will be the topic of some soon coming publications.