

Machine learning emulation of urban land surface processes

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RESEARCH ARTICLE

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Special Section:Machine learning application to
Earth system modeling**Key Points:**

- Ensemble mean of several urban land surface models is accurately emulated using a neural network emulator
- The emulator reduces computational time and complexity compared to a typical urban land surface model
- Coupled to a numerical weather model, the emulator produces accurate and stable forecasts

Supporting Information:Supporting Information may be found in
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Machine Learning Emulation of Urban Land Surface Processes

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Abstract Can we improve the modeling of urban land surface processes with machine learning (ML)? A prior comparison of urban land surface models (ULSMs) found that no single model is “best” at predicting all common surface fluxes. Here, we develop an urban neural network (UNN) trained on the mean predicted fluxes from 22 ULSMs at one site. The UNN emulates the mean output of ULSMs accurately. When compared to a reference ULSM (Town Energy Balance; TEB), the UNN has greater accuracy relative to flux observations, less computational cost, and requires fewer input parameters. When coupled to the Weather Research Forecasting (WRF) model using TensorFlow bindings, WRF-UNN is stable and more accurate than the reference WRF-TEB. Although the application is currently constrained by the training data (1 site), we show a novel approach to improve the modeling of surface fluxes by combining the strengths of several ULSMs into one using ML.

Plain Language Summary Climate change and densely populated cities make the task of urban weather and climate prediction more and more critical to our society. In this study, we use machine learning to improve the accuracy and efficiency of models predicting urban weather. We find great potential to use these types of machine learning models both as standalone tools and integrated into complex weather models.

1. Introduction

Land surface models (LSM) parameterize energy exchanges between the surface and the atmosphere, providing the lower boundary conditions (e.g., radiative and turbulent heat fluxes) to atmospheric models (Stensrud, 2007). For urban areas, ULSMs (urban LSMs) are currently employed in some operational numerical weather prediction (e.g., Bengtsson et al., 2017; Seity et al., 2011) and global climate models (e.g., Hertwig et al., 2021; Oleson et al., 2011) at the higher spatial resolution end, but there is a growing need for broader adoption as they are fundamental to the delivery of integrated urban services (Baklanov et al., 2018; Grimmond et al., 2020). The complexity of ULSMs varies from simple assumptions (e.g., characterizing an impervious slab) to models that consider the 3D geometry of buildings with varying heights and material characteristics (Grimmond et al., 2009, 2010). This higher complexity, however, often comes at the cost of a greater number of site-specific input parameters and increased computational cost, which does not necessarily translate into improved results (Grimmond et al., 2011).

In recent years, machine learning (ML) techniques have shown potential in several areas of meteorology (e.g., Bolton & Zanna, 2019; Krasnopolsky et al., 2013; Nowack et al., 2018; Rasp & Lerch, 2018; Rasp et al., 2018). A key limitation of these techniques, however, is the need for large amounts of training data which, in urban meteorology, are often scarce.

One alternative to this is the creation of ML emulators (i.e., statistical surrogates of their physical counterparts) to improve the computational performance for a trade-off in accuracy (Meyer et al., 2021). Although emulators seek to improve the computational performance of current physical parameterizations, they offer no improvement in accuracy as surrogate models are, at best, as good as the data they are trained on. In urban land surface modeling, speed is, however, not such a limitation; unlike processes such as radiative transfer where the fundamental processes are well understood but computational cost is the primary limiting factor (Meyer et al., 2022), most current ULSMs are reasonably fast but require several input parameters. Furthermore, previous comparisons (Grimmond et al., 2010, 2011) found that no individual ULSM is best at predicting all the main surface fluxes such as short- and longwave radiation, and turbulent sensible and latent heat fluxes. Although an obvious solution to this issue may be mitigated by running an ensemble of ULSMs coupled to a weather (or climate) model

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and use it to improve predictions, this is technically challenging to implement and hard to defend given the multi-fold increase in the computational cost resulting from running multiple ULSMs at once. Moreover, given the complexity of ULSMs, their availability, and the number of specific parameters needed to make realistic simulations, ULSMs often need a specialized team of people while an ML emulator may learn the behavior of an ensemble mean and be a cheaper and easier alternative to run.

Here, we seek to develop an emulator of urban land surface processes and evaluate whether the strengths of multiple ULSMs can be combined to improve both accuracy and computational performance. The specific goals of this paper are:

1. To develop an ML emulator of urban land surface processes trained on the outputs of several ULSMs
2. To evaluate the emulator's accuracy and computational performance
3. To couple the developed ML emulator to a numerical weather model and to evaluate its accuracy and stability

To our knowledge, this is the first attempt to emulate a ULSM. In the following sections, we introduce the general problem of urban land surface modeling with details about data and methods used to develop the emulator (Section 2) and analyze the results (Section 3) before concluding with a summary and ideas for further work (Section 4).

2. Methods

2.1. General Problem

At the core of ULSMs is the concept of surface energy balance (SEB), a general statement of energy conservation with applications to surfaces and volumes of all temporal scales (Oke et al., 2017). Physically, it describes the heating (or cooling) of a surface (Figure 1). Mathematically, it can be stated as:

$$\frac{dQ_s}{dt} = Q^* - Q_H - Q_E, \quad (1)$$

where dQ_s/dt is rate of change in thermal energy stored in a surface by conduction with Q_s the heat storage; $Q^* = (S^\downarrow - S^\uparrow) + (L^\downarrow - L^\uparrow)$ is the surface net all-wave radiation flux density from downwelling (\downarrow) and upwelling (\uparrow) shortwave (S) and longwave (L) radiation; the convective heat flux densities are Q_H the turbulent sensible and Q_E the turbulent latent (or evaporative). Anthropogenic heat fluxes, the additional energy fluxes associated with human activities, if not simulated or prescribed, may be assumed to be zero or minimal in ULSMs (e.g., in low-density residential areas). The horizontal advection of heat and moisture is generally ignored or parameterized by ULSMs but implicitly included when coupled to weather models. ULSMs generally solve a prognostic equation in the form of Equation 1 to predict the evolution of upwelling short- and longwave radiation flux density, sensible and latent heat flux density, forced by downwelling short- and longwave radiation flux density, air temperature and humidity, atmospheric pressure, wind speed and direction and liquid (or solid) precipitation.

2.2. Urban Neural Network

The urban neural network (UNN) developed here is based on the multilayer perceptron (MLP; Bishop, 2006; Goodfellow et al., 2016), one of the simplest types of neural networks (NNs). The MLP-based UNN (Figure 2) is set up to predict upwelling short- and longwave radiation flux density and turbulent sensible and latent heat flux density (Table 1) at time $t + 1$ from inputs at time t of common meteorological variables such as dry-bulb air temperature and humidity, as well as the cosine of solar zenith angle μ_0 and model timestep length Δt (Table 1). Both μ_0 and Δt are used to allow the UNN to run over different grid points at different spatial and temporal resolutions when coupled to the weather model (Section 2.4). Specifically, μ_0 is used instead of latitude, longitude, and local time to reduce the number of features required by the UNN, and Δt to dynamically vary the timestep length, matching that used by the weather model. The surface temperature T_s is used rather than the upwelling longwave radiation L^\uparrow to mimic a physical system whereby T_s is used as a state between different timesteps and thus provide the initial condition at each new inference timestep (Figure 2). The UNN is implemented in TensorFlow (Abadi et al., 2015) version 2.6.2 (TensorFlow Developers, 2021c) and configured with two hidden layers,

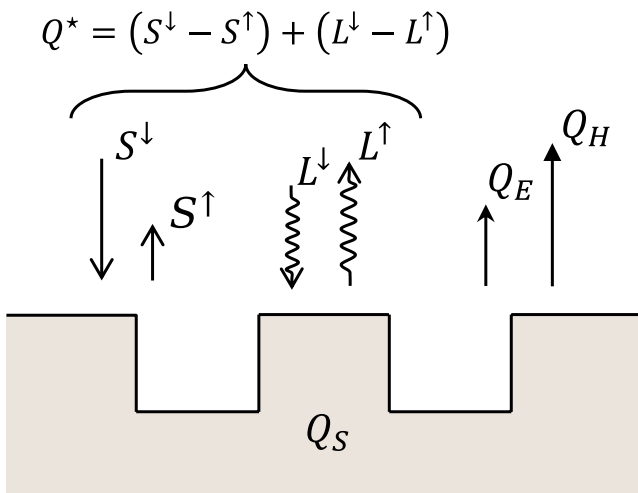


Figure 1. Conceptual sketch of surface energy balance exchanges (ignoring advection, vegetation, and anthropogenic heat flux) for a clear-sky day with arrows indicating the direction of fluxes relative to the surface. The shortwave flux is zero at night as the Sun's rays are below the horizon. The heat transfer processes are (left to right) radiative and convective. Other terms are defined in the text and Table 1.

each having 256 neurons, rectified linear unit (ReLU) activation function, and Adam optimizer (Kingma & Ba, 2015) with mean squared error as its optimization function. This configuration is deemed optimal after conducting a hyperparameter optimization of several configurations (Table S1 in Supporting Information S2) and visually inspecting the results.

2.3. Town Energy Balance

To compare the UNN to a baseline, here we use the Town Energy Balance (TEB; Masson, 2000) model, a single-layer ULSM characterizing city areas based on building roofs, walls, roads, and vegetation, and assuming buildings create an infinite street canyon (Masson, 2000). TEB is chosen as it is a mature, widely used ULSM, extensively evaluated (e.g., Lemonsu et al., 2004; Masson et al., 2002; Pigeon et al., 2008), and available both offline (Meyer, Schoetter, Masson, & Grimmond, 2020) and online (i.e., coupled to weather models; e.g., Hamdi et al., 2012; Lemonsu & Masson, 2002; Meyer, Schoetter, Riechert, et al., 2020). Here we use the TEB software (Meyer, Schoetter, Masson, & Grimmond, 2020) version 4.1.2 (Masson et al., 2021) and refer to it as TEB. Similar to the UNN, TEB inputs include typical meteorological variables at time t , such as dry-bulb air temperature and humidity (Table 1), to predict common surface energy balance variables at time $t + 1$ (Table 1).

2.4. Weather Research and Forecasting (WRF) Coupling

Both TEB and the UNN are coupled to the weather model WRF (Skamarock et al., 2019) in WRF-CMake (Riechert & Meyer, 2019b) version 4.2.2 (Riechert & Meyer, 2021) as it simplifies WRF-related development, configuration, and build-processes. Implementation details of WRF-TEB are provided in Meyer, Schoetter, Riechert, et al. (2020). Variables used in the WRF-UNN and WRF-TEB coupling are similar; however, as friction velocity u_* data are not provided in either observations or most ULSMs (Figure S1 in Supporting Information S1), it is not part of the UNN (Section 2.2) and thus ignored in WRF-UNN.

Porting the UNN to WRF is made seamless by relying on the available C application programming interface (API) provided with TensorFlow (TensorFlow Developers, 2021a). We choose the lightweight version of TensorFlow, TensorFlow Lite (TensorFlow Developers, 2021b) as: (a) it has CMake support, which makes the integration in WRF-CMake straightforward and allows sharing of project build options in WRF-CMake, and (b) it has a very succinct and accessible API (compared to TensorFlow library C API), that makes the Fortran binding used in the coupling easy to write.

To perform the actual coupling, the UNN is exported to a TensorFlow Lite file from Python. To enable the UNN in WRF, the TFLite Fortran binding (tflite.f90; Figure 3a) and the UNN surface module (module_sf_unn.F; Figure 3) are written. The former is used to interface with the TFLite C API and the latter to initialize inputs (Table 1) and run the UNN to generate outputs (Table 1) which are passed to WRF for the next timestep.

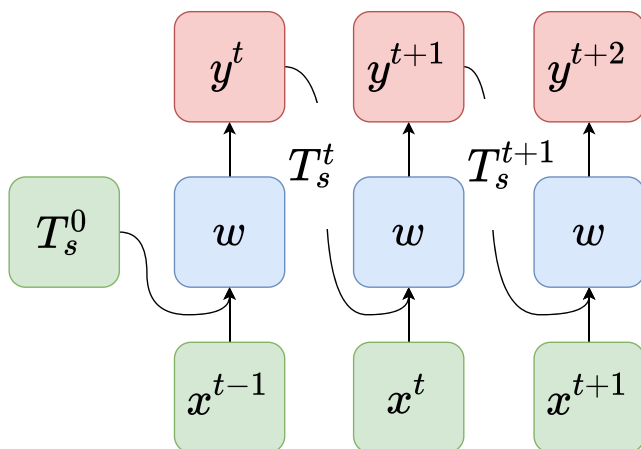


Figure 2. The trained urban neural network (UNN) is used to predict outputs y (Table 1) at time $t + 1$ from inputs x (Table 1) at time t using trained weights w . The surface temperature T_s from a previous timestep provides the initial condition at each new inference.

2.5. Data and Model Setup

Grimmond et al. (2011)'s urban comparison study evaluated the accuracy of 32 ULSMs (or different configurations) from a wide range of international modeling groups (Table S2 in Supporting Information S2) using directly observed fluxes in Preston, a suburban area of Melbourne (Australia). Site information to configure ULSMs, released to participants in four Stages, gives increasing detail (Table S3 in Supporting Information S2). For each

Table 1
Inputs and Outputs From Data Sets and Models Used to Conduct the Simulations

Symbol	Name	Unit	MEM	TEB ^a	WRF-TEB ^a	UNN	WRF-UNN	Derived as
Inputs								
T	Dry-bulb air temperature	K	✓	✓	✓	✓	✓	-
q	Specific humidity	kg kg ⁻¹	✓	✓	✓	✓	✓	-
p	Atmospheric surface pressure	Pa	✓	✓	✓	✓	✓	-
S^{\downarrow}	Downwelling shortwave radiation flux density	W m ⁻²	✓	✓ ^b	✓ ^b	✓	✓	-
L^{\downarrow}	Downwelling longwave radiation flux density	W m ⁻²	✓	✓	✓	✓	✓	-
u	Zonal component of wind velocity	m s ⁻¹	✓ ^c	✓ ^c	✓	✓	✓	-
v	Meridional component of wind velocity	m s ⁻¹	✓ ^c	✓ ^c	✓	✓	✓	-
RR	Rainfall rate	kg m ⁻² s ⁻¹	✓	✓	✓	✓	✓	-
t_{local}	Local time	s	✓	✓	✓	-	-	-
φ	Latitude	deg	✓	✓	✓	-	-	-
λ	Longitude	deg	✓	✓	✓	-	-	-
μ_0	Cosine of solar zenith angle	rad	-	-	-	✓ ^b	✓	-
Δt	Timestep length	s	✓	✓	✓	✓	✓	-
Outputs								
S^{\uparrow}	Upwelling shortwave radiation flux density	W m ⁻²	✓	✓	-	✓	✓	-
L^{\uparrow}	Upwelling longwave radiation flux density	W m ⁻²	✓	✓	-	-	D	$\epsilon \sigma T_s^4$
T_s	Surface (skin) temperature	K	-	✓	✓	S	S	$[L^{\uparrow}/(\epsilon \sigma)]^{1/4}$
Q_H	Turbulent sensible heat flux density	W m ⁻²	✓	✓	✓	✓	✓	-
Q_E	Turbulent latent heat flux density	W m ⁻²	✓	✓	✓	✓	✓	-
E	Evaporation mass flux density	kg m ⁻² s ⁻¹	-	✓	✓	-	D	Q_E / L_v
Q_S	Heat Storage	J m ⁻²	-	✓	✓	-	D	Equation 1
α	Surface albedo	1	C	C	C	-	D	$S^{\uparrow}/S^{\downarrow}$
ϵ	Surface emissivity	1	C	C	C	-	-	-
w_s	Mass mixing ratio of water vapor	kg kg ⁻¹	-	✓	✓	-	U	-
u_*	Shear (friction) velocity	m s ⁻¹	-	✓	✓	-	U	-

Note. Multi-model Ensemble Mean (MEM). Depending on the model or data set used, data may be unavailable/not-applicable (-), available/outputted (✓), derived (D), constant (C), unmodified (U), state (S). For computations between upwelling longwave radiation flux density L^{\uparrow} and surface temperature T_s a constant emissivity (ϵ) of 0.97 as reported in Coutts et al. (2007b) is used. The latent heat of vaporization L_v is assumed to be constant with a value of 2.464 MJ kg⁻¹ which is applicable to 15°C (Oke et al., 2017). ^aAdditional inputs and outputs are given in namelists. ^bTEB requires direct and diffuse; these are computed using pvlb (Holmgren et al., 2018) version 0.9.0 (Holmgren et al., 2021) but given directly as-is in WRF. ^cWind speed and direction are used instead of, and derived from the zonal and meridional components of wind velocity using MetPy version 1.1.0 (May et al., 2021).

Stage, groups returned their model computed surface energy balance fluxes. The main data sets, with local time stamps (UTC + 10, i.e., 10-h ahead of Coordinated Universal Time), are:

1. *Morphological parameters* (MP): provided in the four Stages, characterizing the surface around the observation site (Grimmond et al., 2011 Table 2, and our Table S3 in Supporting Information S2).
2. *Meteorological Forcing* (MF; Grimmond et al., 2021): continuous gap-filled 30-min averages with a period ending timestamp (i.e., 10:30 is 10:01–10:30) of meteorological variables at 40 m above ground level (agl) between 12 August 2003 13:30 and 28 November 2004 23:00 (Figure 4; Table 1).
3. *Multi-model output* (MO; Grimmond et al., 2013): continuous outputs, from 32 models or model-configurations between 13 August 2003 00:00 and 27 November 2004 23:30 reported in four separate Stages for upwelling short- and longwave radiation flux density, and turbulent sensible and latent heat flux density (Table 1).

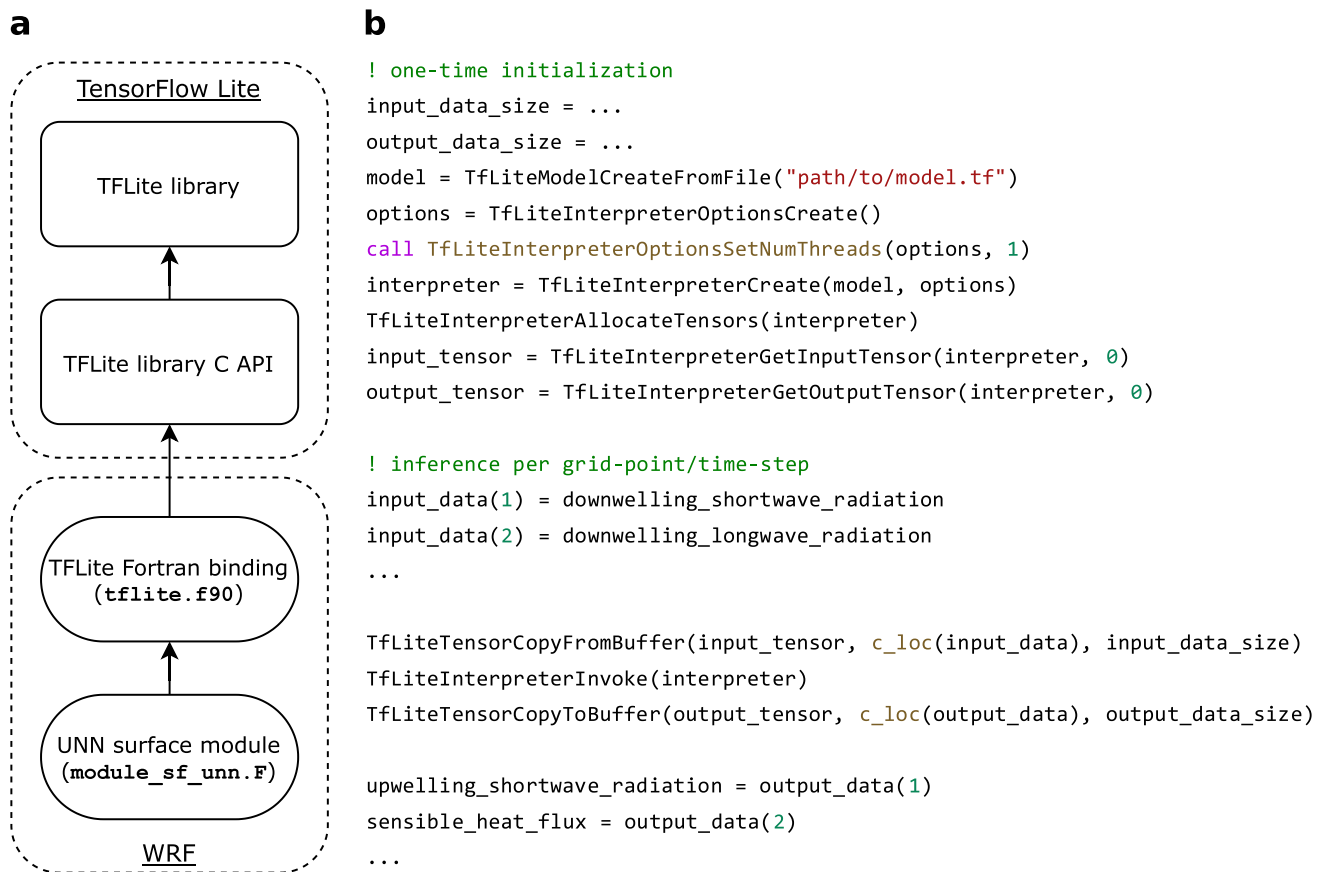


Figure 3. Call to Tensorflow Lite (TFLite) C API from WRF as implemented for this study. (a) TFLite integration: the Fortran interface module `tflite.f90` is used in WRF to bind to the TFLite C API, which is used by the UNN surface module `module_sf_unn.F` to initialize and run the neural network. (b) Example of TFLite Fortran binding (simplified from UNN surface module) use: first, a one-time initialization to load the TFLite model, configure its settings, and allocate input and output tensors is performed. Before each inference, input quantities (e.g., downwelling shortwave radiation) are stored in the input tensor in the expected order. Similarly, inference outputs are returned as output tensors from which individual quantities are accessed. Other pre- and post-processing steps such as normalization and error handling are omitted. See `models/wrf-unn/phys/module_sf_unn.F` and `models/wrf-unn/phys/module_sf_unn.F` in Meyer (2021) for actual code.

4. *Observations* (OBS; Grimmond et al., 2021): 30-min average fluxes with period ending timestamp measured at 40 m agl between 13 August 2003 00:00 and 27 November 2004 23:30. Methods to obtain observed fluxes are given in Coutts et al. (2007a, 2007b). This data set has the same fluxes as the MO data set but with observational gaps (~39% of MO; purple Figure 4a).

Here, a visual inspection of the MO data set for all Stages (Figure S2 in Supporting Information S1) is used to remove ULSMs not simulating the turbulent latent heat flux density (8 ULSMs) or showing outliers (2 ULSMs), leaving 22 ULSMs (Figure S3 in Supporting Information S1). The MO data set is used to compute the ensemble mean, hereafter referred to as the multi-model ensemble mean (MEM). To make evaluations consistent between MEM, UNN, and TEB, these are conducted for periods spanning 13 August 2003 00:00 and 27 November 2004 23:30 as defined in MEM totaling 22,704 30-min samples. For any given data set, the test fraction is the periods with OBS available (i.e., 39% of MEM; number of samples $N = 8,866$; purple, Figure 4a) and the training fraction (used by the UNN; see point 2 below) for the remaining periods (i.e., 61% of MEM; $N = 13,838$; black, Figure 4a). Evaluation metrics (Section 2.6) are calculated for the test fraction, with results (Section 3) using all samples except for the upwelling shortwave radiation flux density as this is zero at nighttime (i.e., daytime: OBS $> 2 \text{ W m}^{-2}$, $N = 4,272$).

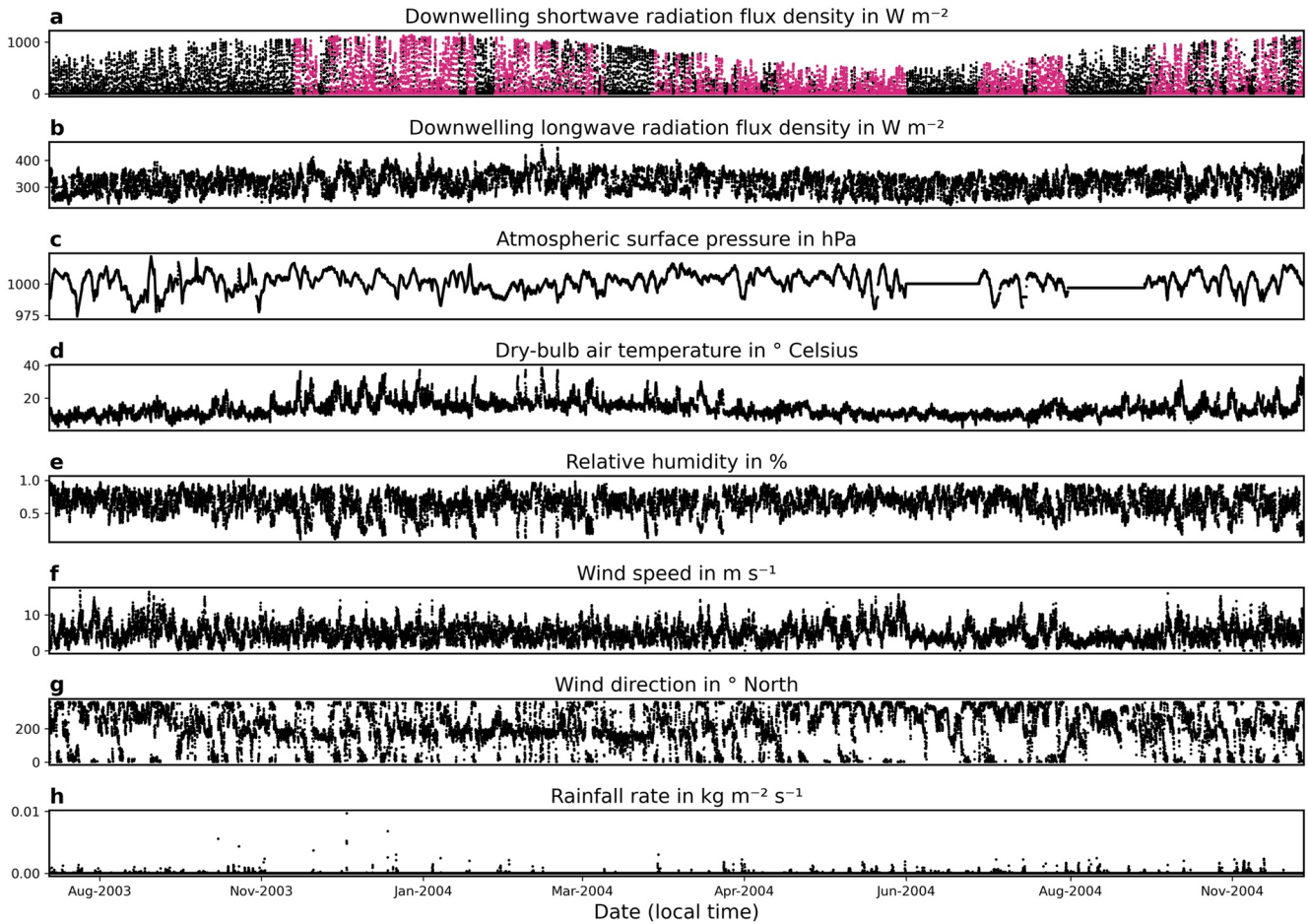


Figure 4. Observed meteorological forcing data (30-min, Section 2.5): (a) downwelling shortwave radiation flux density with observed fluxes (i.e., test fraction) shown in purple, (b) downwelling longwave radiation flux density, (c) atmospheric surface pressure, (d) dry-bulb air temperature, (e) relative humidity, (f) wind speed and (g) wind direction, and (h) rainfall rate. The wind speed and direction are computed using MetPy version 1.1.0 (May et al., 2021) from the zonal and meridional components of wind velocity. The relative humidity is computed using PsychoLib (Meyer & Thevenard, 2019) version 2.5.0 (Meyer & Thevenard, 2020) from the dry-bulb air temperature, specific humidity, and atmospheric surface pressure. Local time is 10-hr ahead of Coordinated Universal Time (UTC + 10).

Model-specific setups are as follows:

1. TEB uses morphological parameters from MP for the four Stages (Table S3 in Supporting Information S2) forced with MF. TEB is run with 5-min (300-s) timesteps (from 13 August 2003 00:00 to 27 November 2004 23:30) after linear interpolation of the 30-min MF data set (e.g., 00:00, 00:05, ...) to predict the next 5-min (e.g., 00:05, 00:10, ...). The last 5-min sample of each 30-min period (e.g., 00:30) is used in analyses (Section 3). From the evaluation of TEB outputs at all Stages, Stage 4 is selected as it has the smallest errors (Appendix A).
2. The UNN is trained with MF as inputs and MEM from Stage 2 as outputs (Table 1) using the training fraction. Stage 2 is selected as it offers the 'best' tradeoff between complexity (i.e., number of parameters used to configure the 22 ULSMs; Table S3 in Supporting Information S2) and accuracy (Appendix A). Prior to training, the surface temperature T_s is derived from the MEM upwelling longwave radiation flux density L^{\uparrow} assuming a constant emissivity (Table 1). To allow the UNN to be used with different timestep lengths, nine linearly interpolated copies of both inputs and outputs are made (with 1, 2, 5, 10, 20, 60, 120, 300, and 600-s timesteps), each derived from the 30-min data, and concatenated together with the original. A random subset corresponding to the same number of samples included with the 30-min data ($N = 13,838$) is selected in each copy to keep the number of training samples across the linearly interpolated copies equal. Thus, the total number of samples used for training the UNN is 138,380 (i.e., ten times the original 30-min data). Of this, 25% are randomly reserved for the early stopping mechanism. For inference, the UNN is forced with

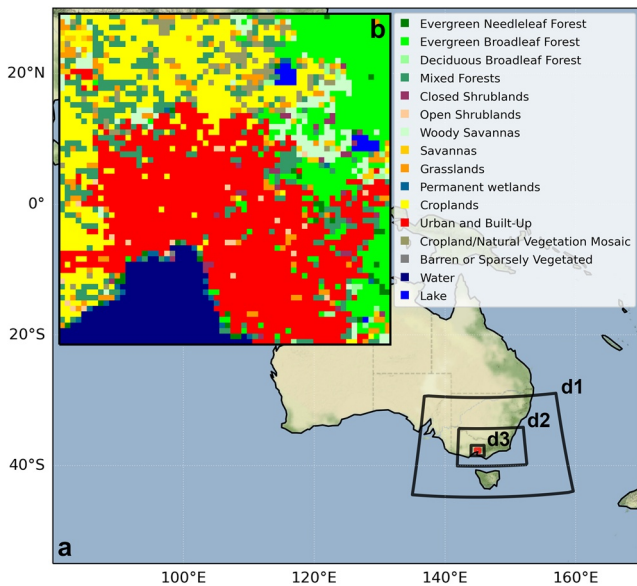


Figure 5. Study area (a) within Australia and the four nested domains (d1–d3 and innermost, red) used in online simulations, and (b) innermost domain (1 km horizontal grid spacing) with WPS MODIS 30 arc-sec land cover/use (UCAR, 2019). The UNN and TEB are run for “urban” (red) grid cells in WRF, assuming land cover fractions of 0.445 building, 0.38 vegetation, and remainder non-building impervious. Sources: map features by Natural Earth Vector (Kelso & Patterson, 2009) are in the public domain. Map tiles by Stamen Design (2021), under Creative Commons Attribution 3.0 license (CC BY 3.0). Data from OpenStreetMap (OpenStreetMap contributors, 2017), under Open Data Commons Open Database License (ODbL).

5-min MF (12 August 2003 23:30 and 27 November 2004 23:30) derived by linearly interpolating the 30-min intervals to be consistent with TEB. As UNN outputs (Table 1) include T_s rather than L^\dagger used in evaluations, UNN outputs are post-processed to derive L^\dagger from T_s assuming a constant emissivity (Table 1). The stochastic nature of the multilayer perceptrons is assessed by repeating the training (and inference) 100 times, each with a different random seed. At each iteration (a) for each UNN output variable (S^\dagger , L^\dagger , Q_H , Q_E ; Table 1), the normalized mean absolute error (nMAE; Section 2.6) is computed using the ‘true’ MEM and UNN-predicted samples for the whole period (i.e., both train and test fractions) and (b) the mean nMAE (nMAE) is computed as $0.25 (\text{nMAE}_{S^\dagger} + \text{nMAE}_{L^\dagger} + \text{nMAE}_{Q_H} + \text{nMAE}_{Q_E})$. The UNN with the median nMAE from the 100 iterations (Figure S4 in Supporting Information S1) is taken as the representative UNN and used in analyses (Section 3). Thus, all UNN-relevant metrics (Section 2.6) are computed using results from the UNN with the median nMAE.

3. The coupled WRF-TEB and WRF-UNN simulations are set up with four nested domains (Figure 5), generated with GIS4WRF (Meyer & Riechert, 2019) version 0.14.4 (Meyer & Riechert, 2020) and processed using WPS-CMake (WRF Preprocessing System) version 4.1.0 (Riechert & Meyer, 2019a). Both TEB and the UNN are run for the innermost domain (Figure 5b) with a 5-s timestep centered on the Preston measurement tower. The innermost domain with 1 km horizontal grid spacing has a 66 m vertical grid spacing close to the surface, increasing with height. As model buildings are assumed to be within the ground (Meyer, Schoetter, Riechert, et al., 2020), the flux tower sensors at 40 m agl is 33.6 m above the model surface (as mean building height = 6.4 m, Table S3 in Supporting Information S2). WPS MODIS land use data (UCAR, 2019) are used as one urban class with the same urban and vegetation fractions (i.e., all grid cells) for consistency between TEB and UNN simulations. Stage 4 parameters (Table S3 in Supporting Information S2) are used in both WRF-TEB, and TEB-offline runs. The European Centre for Medium-Range Weather Forecasts (ECMWF) Cycle 28r2 analysis (ECMWF, 2004) data are used to provide the initial and boundary conditions. Other parameters used to configure WRF and WPS are given in Table S4 of Supporting Information S2. Simulations are run for summer (23 December 2003 10:00–27 December 2003 10:00) and winter (25 June 2004 10:00–31 June 2004 04:00) periods, with evaluations using 65 hr in summer (24 December 2003 14:30–27 December 2003 07:30) and 98.5 hr in winter (26 June 2004 21:00–30 June 2004 23:30) to allow some model spin-up; giving the longest continuous observation evaluation periods in the two seasons. Instantaneous WRF fluxes at each 5-min interval (e.g., 00:00, 00:05, ...) are averaged to 30-min time ending values for comparison with OBS.

2.6. Evaluation Metrics

To assess the simulations, statistics are computed between ‘true’ y^t and ‘predicted’ \hat{y}^t samples at time t for $1..N$ timesteps. The metrics used are: mean bias ($\text{MB} = 1/N \sum_{t=1}^N \hat{y}^t - y^t$), mean absolute error ($\text{MAE} = 1/N \sum_{t=1}^N |\hat{y}^t - y^t|$), mean absolute error normalized by mean absolute “true” flux $|y^t|$ (hereafter referred to as the normalized mean absolute error, $\text{nMAE} = 100\% \left[\frac{\text{MAE}}{|y^t|} \right]$) and standard deviation of the error ($\text{SDE} = \sqrt{\frac{1}{N} \sum_{t=1}^N \left[(\hat{y}^t - y^t) - \overline{(\hat{y}^t - y^t)} \right]^2}$). Depending on the evaluation type, the ‘true’ samples y^t are from either OBS or MEM and predicted samples \hat{y}^t are from either MEM, UNN or TEB outputs (Section 2.5).

Table 2

Observed Flux Densities (Upwelling Shortwave S^{\uparrow} and Longwave L^{\uparrow} Radiation, and Turbulent Sensible Q_H and Latent Q_E Heat) and Modeled (UNN, MEM, and TEB) Evaluation Metrics (Section 2.6) for N 30-Min Periods With the Lowest nMAE (Bold) per Flux Indicated per Data Cohort

	S^{\uparrow}	L^{\uparrow}	Q_H	Q_E	S^{\uparrow}	L^{\uparrow}	Q_H	Q_E	S^{\uparrow}	L^{\uparrow}	Q_H	Q_E
Observed	Mean ($W\ m^{-2}$)											
16 months	58	390	40	34	-	-	-	-	-	-	-	-
65.5 hr in summer	87	420	100	46	-	-	-	-	-	-	-	-
82 hr in winter	41	350	-3.9	22	-	-	-	-	-	-	-	-
Simulated	MB ($W\ m^{-2}$)				MAE ($W\ m^{-2}$)				nMAE (%)			
16 months (13 August 2003 00:00–27 November 2004 23:30; $N = 8,866$, except $S^{\uparrow} N = 4,272$)												
MEM	-4.7	-0.39	-0.67	1.3	5.3	4.0	20	19	9.2	1.0	33	51
UNN	-1.7	-4.9	-6.9	7.1	5.5	7.8	21	20	9.4	2.0	36	54
TEB	3.0	-19	-18	-3.8	5.1	20	30	25	8.7	5.2	51	68
65.5 hr in summer (24 December 2003 14:30–27 December 2003 07:30; $N = 131$, except $S^{\uparrow} N = 73$)												
Offline: MEM	-6.6	0.4	-18	0.53	7.8	4.6	29	24	9.0	1.1	27	46
UNN	-3.2	0.65	-9.8	9.3	6.3	5	24	25	7.2	1.2	23	47
TEB	2.1	-28	-22	-11	6	31	38	30	6.9	7.3	35	57
Online: WRF-UNN	-5.8	14	15	-4.7	9.5	18	38	26	11	4.2	35	49
WRF-TEB	-2.1	-11	-41	-12	8.3	35	53	34	9.6	8.2	49	64
82 hr in winter (26 June 2004 21:00–30 June 2004 23:30; $N = 164$, except $S^{\uparrow} N = 56$)												
Offline: MEM	-2.4	-4.3	7.9	6.8	4.2	4.3	13	9.7	10	1.2	27	43
UNN	-0.43	-7.9	-0.24	9.4	4.7	8.0	15	12	11	2.3	33	54
TEB	6.7	-15	-19	10	7.3	15	21	14	17	4.2	45	60
Online: WRF-UNN	-3.3	-1.3	0.53	5.9	8.8	9.3	18	13	21	2.6	38	56
WRF-TEB	3.0	-3.5	-21	8.8	11	16	27	18	28	4.4	59	81

3. Results and Discussion

3.1. Multi-Model Ensemble Mean

First, we assess the trained urban neutral network (UNN) using the test fraction (Section 2.5) of the multi-model ensemble mean (MEM) data set to determine if the UNN captures the main processes in predicting the surface energy balance. A perfect emulator would have all points on the line $x = y$ (Figure 6). The UNN has the highest skill for the daytime upwelling shortwave radiation flux density (Figure 6a): mean bias (MB) is $3.0\ W\ m^{-2}$, standard deviation of the error (SDE) $4.4\ W\ m^{-2}$, mean absolute error (MAE) $4.2\ W\ m^{-2}$, and normalized mean absolute error (nMAE) 7.0%. The UNN-predicted longwave flux (Figure 6b) is slightly poorer (MB/SDE/MAE are $-4.5/6.6/6.4\ W\ m^{-2}$) but with a lower nMAE (1.6%) because of the larger fluxes. The turbulent latent (Figure 6d) heat flux density is more accurately predicted (MB/SDE/MAE are $5.9/13.7/8.6\ W\ m^{-2}$ and nMAE is 32.7%) than the sensible (MB/SDE/MAE are $-6.2/21.4/16.1\ W\ m^{-2}$ and nMAE is 34.2%; Figure 6c) but with larger outliers. This relative ranking is consistent with the extensive ULSM evaluation literature.

3.2. Offline Simulations

Second, we compare the UNN to observed fluxes (OBS) and a version of the widely used ULSM TEB (Section 2.3). Two evaluations are undertaken with each using different meteorological forcing data: (a) observed MF (offline) and (b) coupled to WRF (online). The offline results are analyzed for both the test fraction and the short summer and winter periods (Section 2.5; Table 2). Online simulations (Section 3.3) are only evaluated for the latter two periods.

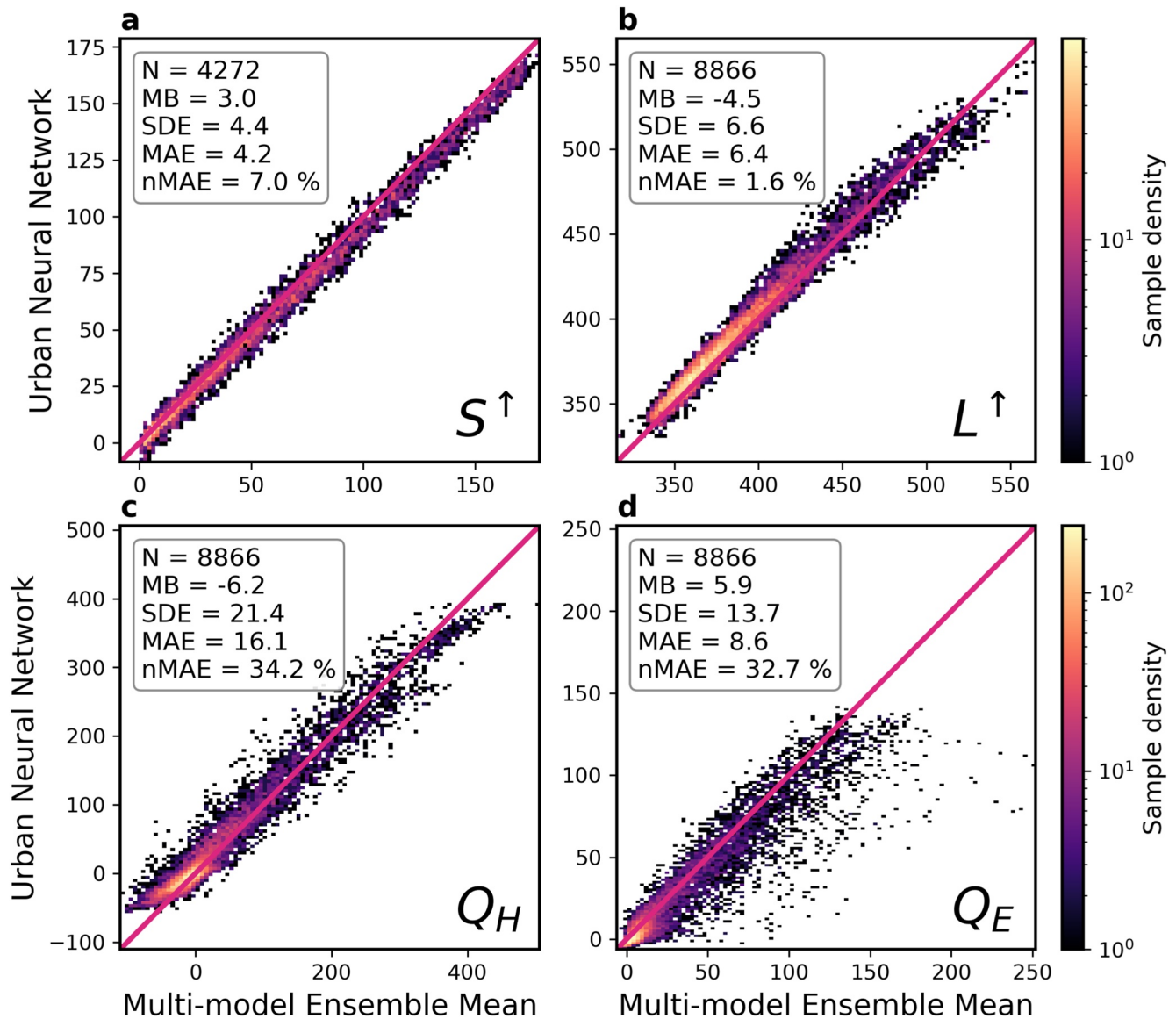


Figure 6. Comparison of UNN to the MEM data, with 1:1 line (red), data density (color), and evaluation statistics (Section 2.6) shown, for 30-min flux densities of (a) daytime upwelling shortwave radiation (S^\uparrow) and (b) 24 hr upwelling longwave radiation (L^\uparrow), turbulent (c) sensible (Q_H), and (d) latent (Q_E) heat. Units are $W m^{-2}$ except for the nMAE percentage (%). Note that axes scales differ between plots.

Relative to OBS, MEM has the lowest biases and errors for all but the upwelling shortwave radiation flux density, where it is outperformed by TEB (Figure 7; Table 2). Similarly, as the UNN captures the main surface processes modeled by the MEM (Section 3.1), its predictions outperform TEB's for all but the upwelling shortwave radiation. The MAE for the upwelling shortwave radiation (Figure 7a; Table 2) for all (MEM\UNN\TEB) is $<6 W m^{-2}$ (Figures 7c–7g; Table 2). The MAE for the longwave (Figure 7b) is larger than for the shortwave, with TEB ($20 W m^{-2}$) having the largest between both MEM and UNN (MEM $4 W m^{-2}$; UNN $7.8 W m^{-2}$). Similarly, the MAE for the turbulent sensible (Figures 7c and 7f) and latent (Figures 7d and 7f) heat flux densities are larger for TEB (30 and $25 W m^{-2}$, respectively) compared to MEM and UNN ($\leq 21 W m^{-2}$, Table 2). The nMAE for the latent is larger than sensible because of its smaller mean (Table 2; Figure 7g). The short summer and winter focal periods are consistent with the 16-month results (Table 2, Figure 8), with generally higher biases and errors for TEB than for either MEM or UNN. However, both MEM and UNN outperform TEB in the winter, notably with better accuracy for upwelling shortwave radiation (Figures 8b and 8i–8n; Table 2).

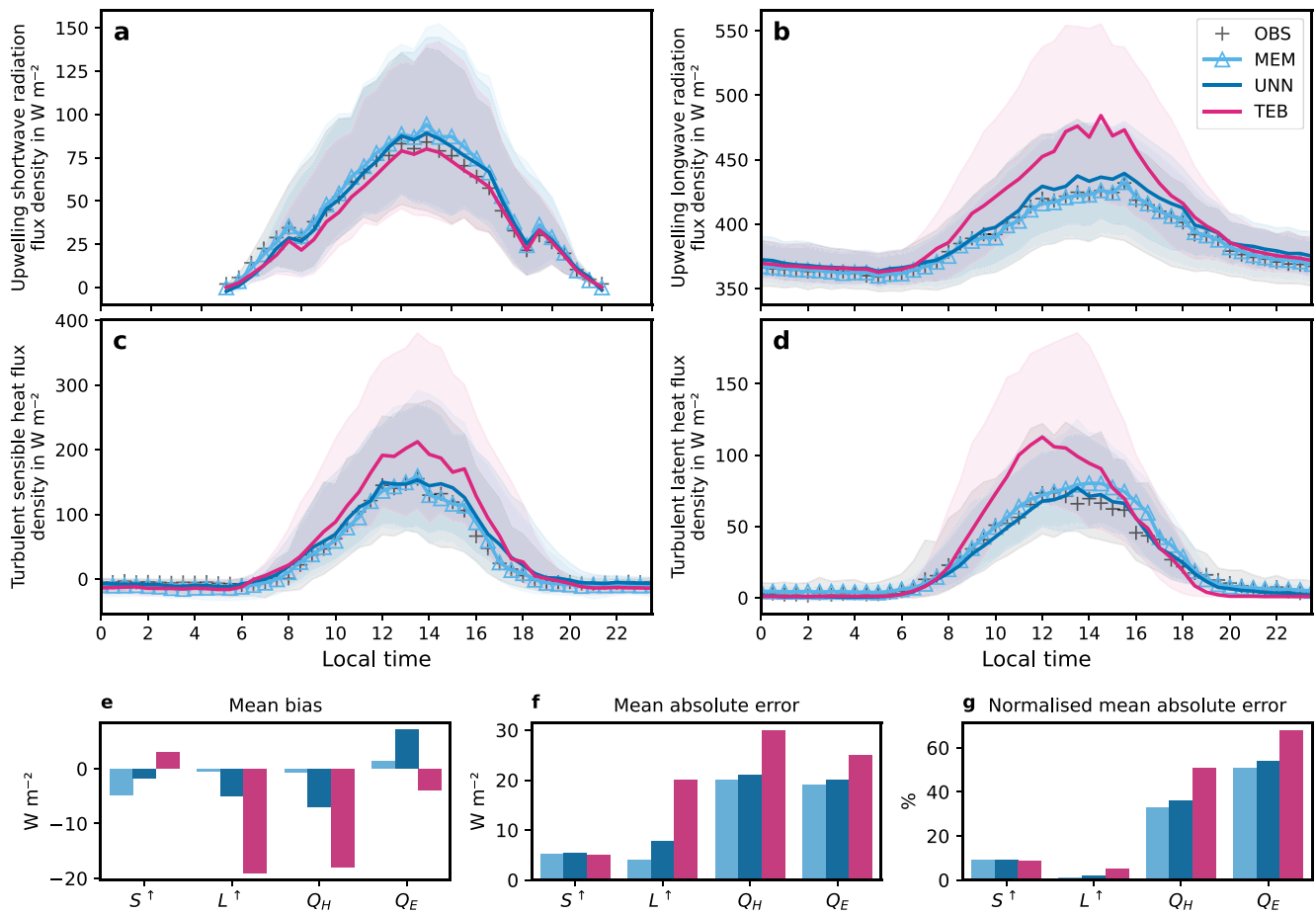


Figure 7. Offline (16-months, $N = 8\,865$) simulated (MEM, UNN, TEB, see text) and observed (OBS) 30-min flux densities (lines) with interquartile range (shading) for (a) upwelling short- (S^\uparrow) (daytime) and (b) longwave (L^\uparrow) radiation, turbulent (c) sensible (Q_H) and (d) latent (Q_E) heat, with (e–g) their respective evaluation metrics (Table 2). Note that the y-axes differ between plots.

3.3. Online Simulations

The online coupled WRF-UNN and WRF-TEB simulation results for the grid cell centered on the measurement site are shown in Figure 9. The numerical stability of WRF-UNN (trained using MEM for Stage 2; Section 2.5) is demonstrated by executing thousands of iterations for hundreds of grid cells without numerical failure (i.e., 2-week, hundreds of domain grid points). The WRF-UNN post-spin-up periods for both winter and summer (Figure 9) capture the general trends of observations. Despite being derived using data from simulations driven with Stage 2 parameters (Table S3 in Supporting Information S2), WRF-UNN has better predictive skills than WRF-TEB (using Stage 4 parameters) for both summer and winter periods (Figure 9). WRF-UNN errors are generally lower than those of WRF-TEB in both seasons for all but the winter upwelling shortwave radiation flux density (Figure 9; Table 2) and generally consistent with the errors shown for offline simulations (Section 3.2).

As online simulations are run for the entire domain, an additional, albeit qualitative, comparison can be made across the spatial domain. The inner domain surface cover is assigned the same land cover fractions (building 0.445, paved/road 0.175, vegetated 0.380) for all ‘urban’ grid cells (d4 red, Figure 5) in both WRF-TEB and WRF-UNN. Given the temporal difference between the two simulations is greatest around midday on 25 December 2003 (Figure 9c), we select this time for the spatial comparisons (Figure 10). Although the simulated upwelling shortwave radiation flux density (Figures 10a and 10b) has a similar pattern across the domain, the longwave (Figures 10c and 10d) in WRF-UNN has a smaller magnitude and spatial range across all the urban grid cells. As a result, the WRF-TEB upwelling longwave radiation flux density is overpredicted by about 100 W m^{-2} (Figure 9e). The warmer WRF-UNN surface temperature can explain the larger turbulent sensible heat flux density at the observational site (Figure 9e) and across the domain (Figures 10e and 10f).

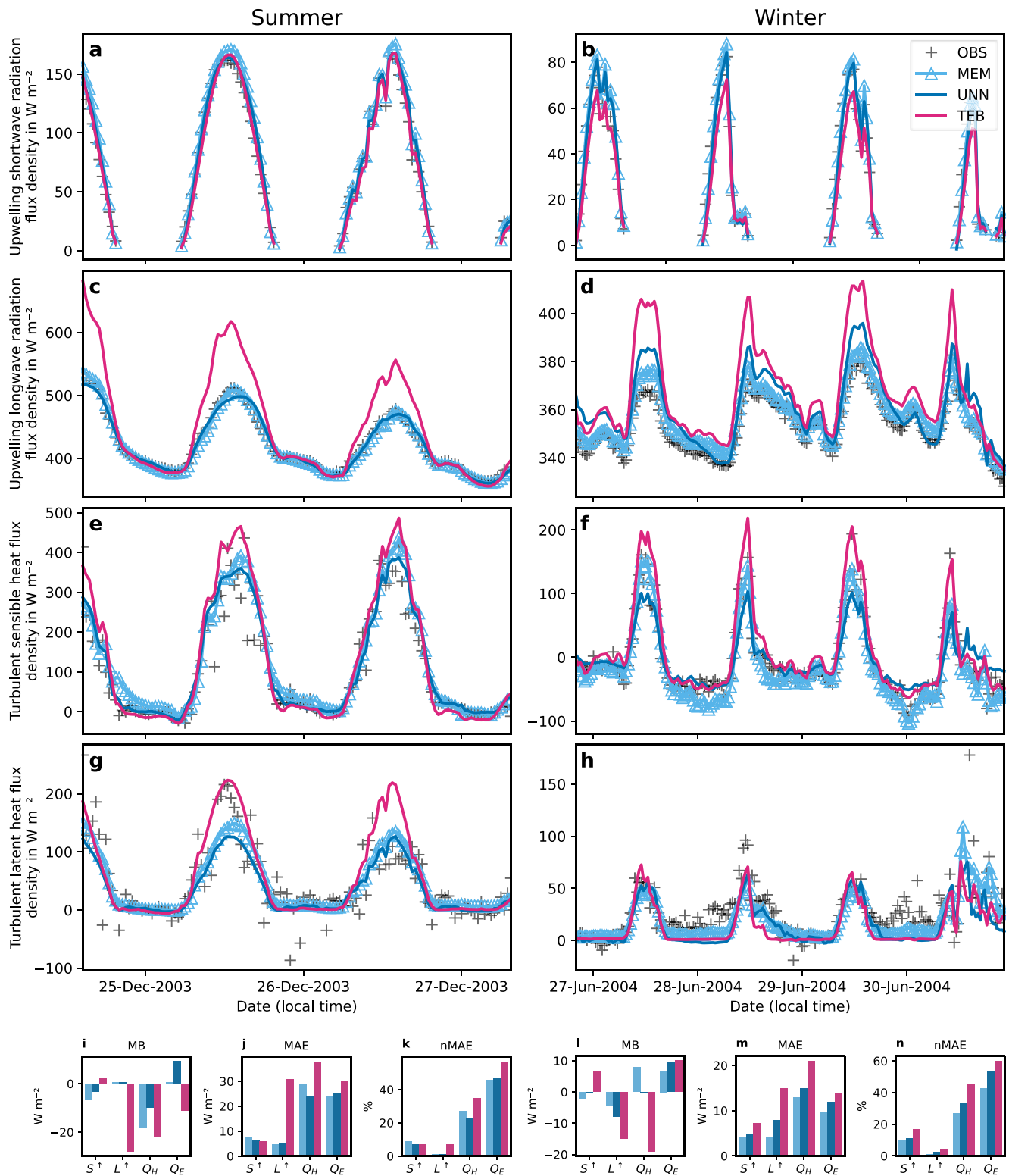


Figure 8. Offline simulated (MEM, UNN, and TEB) and observed (OBS) 30-min flux densities in (a, c, e, g, and i–k) a summer and (b, d, f, h, and l–n) winter period for (a and b) upwelling short- (S^{\uparrow}) and (c and d) longwave (L^{\uparrow}) radiation, turbulent (e and f) sensible (Q_H) and (g and h) latent (Q_E) heat, with (i–n) evaluation metrics (Table 2). Note that the y-axes differ between plots.

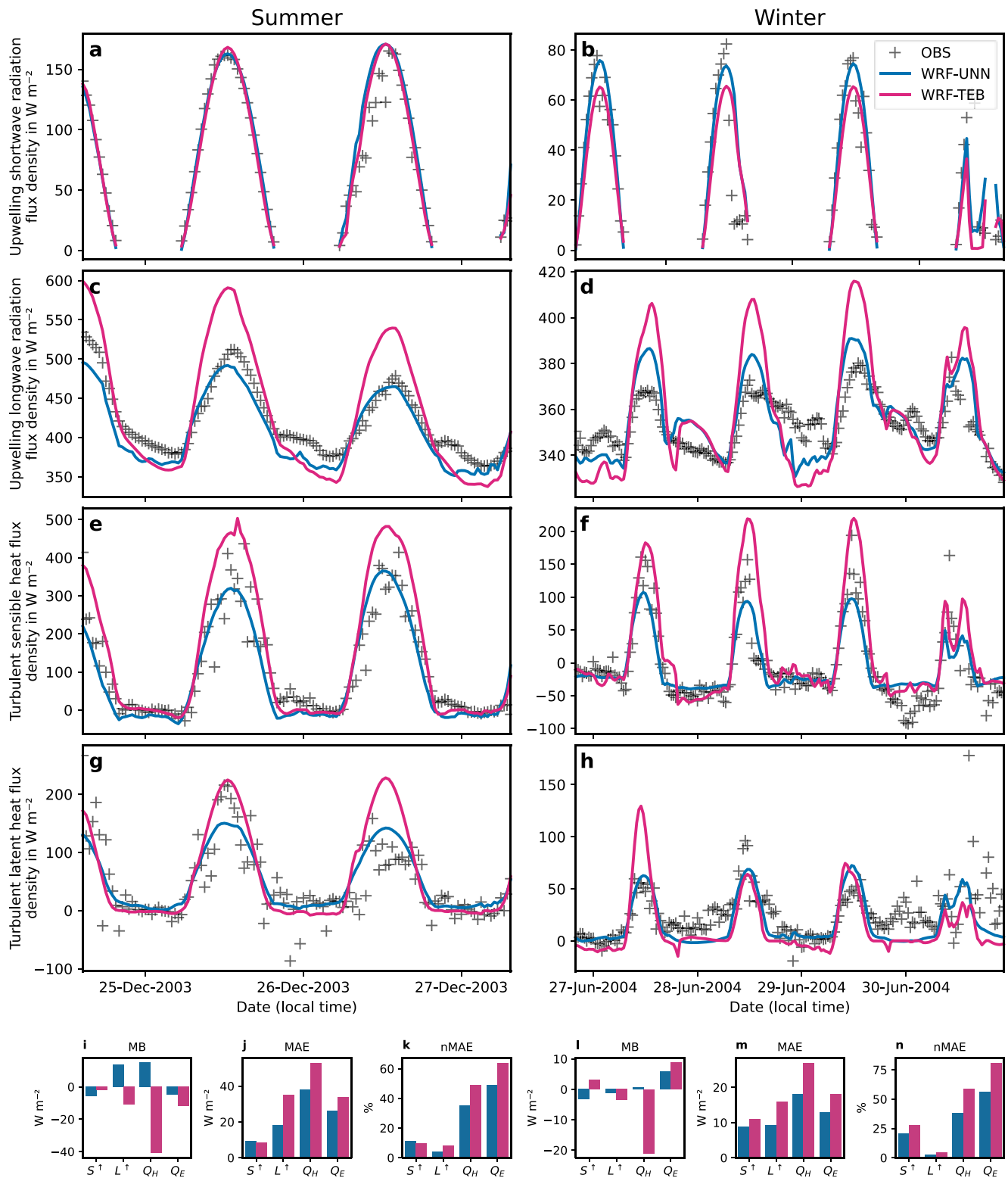


Figure 9. As Figure 8, but for online simulations.

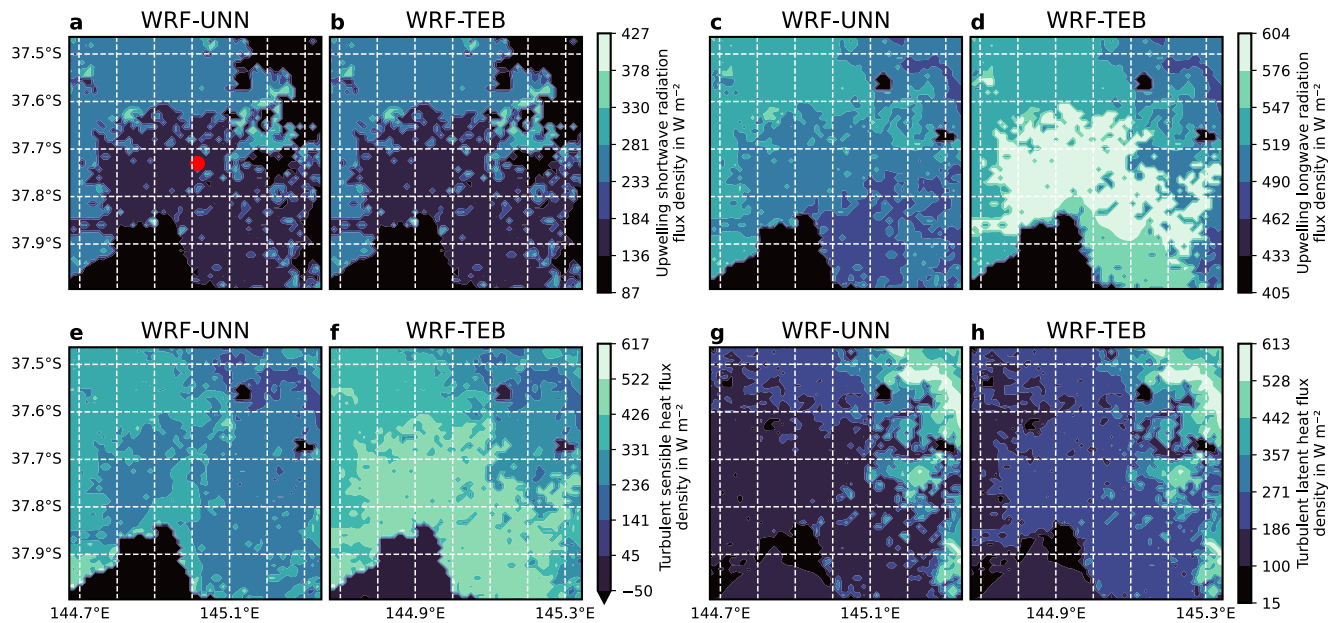


Figure 10. The inner domain (d4, Figure 5) with observation tower (red) for the 30-min average period between 12:00 and 12:30 on 25 December 2003 with flux densities simulated using (a, c, e, and g) WRF-UNN and (b, d, f, and h) WRF-TEB for (a and b) upwelling shortwave (c and d) and longwave radiation, and turbulent (e and f) sensible and (g and h) latent heat.

3.4. Computational Performance

The runtime between offline UNN and TEB simulations is compared based on 100 repeats each for the 16-month period. UNN runs include data normalization and inference using TensorFlow in Python. All runs are conducted on a shared AMD EPYC 7742 CPU node with 32 cores and 124 GiB of system memory. Both TEB and the UNN are configured to run fully single-threaded in a Singularity container running Ubuntu 20.04, GNU Fortran 9.3 compiler, and Anaconda Python 3.9. UNN (0.50 ± 0.0053 s) runs are over one order of magnitude faster than TEB runs (6.0 ± 0.042 s).

4. Conclusion

In this work, we successfully develop a neural network emulator of urban land surface processes (UNN) for offline and online applications. The UNN is trained on the multi-model ensemble mean (MEM) of 22 urban land surface models (ULSMs) for an area of Melbourne, Australia. The accuracy is assessed using flux observations and compared to a well-known ULSM (Town Energy Balance TEB) model. The MEM data are derived from a study with four Stages of increasing complexity (1–4; Appendix A). The UNN is trained using Stage 2 MEM, but compared to the Stage 4 TEB simulations, the latter using more site-specific information.

Compared to MEM, the UNN captures the general variability of surface energy balance fluxes. Relative to the observations, the UNN is more accurate than TEB—or than WRF-TEB when coupled to the Weather Research and Forecasting (WRF) model—while having reduced both computational demands (by over an order of magnitude) and model parameter requirements (i.e., trained using fewer site-specific parameters). Technically, the coupling to WRF is straightforward thanks to WRF-CMake and TensorFlow Lite C bindings.

As the first study to show the development and application of a machine learning (ML) emulator for urban land surface fluxes, we demonstrate its potential to improve the modeling of key surface energy balance fluxes: we combine the strengths of several ULSMs into one and show that such models can be successfully integrated into complex weather models, such as WRF. The development of (coupled) emulators such as WRF-UNN have other advantages compared to ‘more-traditional’ ULSMs such as code optimization at the deployment stage, and integration into different codebases and hardware architectures through common high-level APIs.

Although the current evaluation did not assess, or assume, surface energy balance closure, which is essential for climate applications (Grimmond et al., 2010), further research is needed to assess this before UNNs are used in climate studies. Furthermore, with no variations in urban areas (e.g., land cover fractions, surface parameters, and climate) assessed because of the current lack of multi-site data sets, the natural progression to assess our findings more globally requires data sets currently being developed (Lipson et al., 2020) with or without data augmentation strategies as outlined by Meyer et al. (2021).

Indeed, if MEMs are found to be more accurate than any individual ULSM on a global scale, an ML emulator as described here could help improve both the speed and accuracy of current ULSMs. Aside from the apparent speed-up improvement typical of ML emulators and that of improved accuracy outlined here, ML approaches may also prove helpful in operational Earth system models as the fewer site-specific parameters contained in MEM are easily retrievable and updatable globally using remote sensing techniques.

Appendix A: Stage Selection

Stage 2 data (Table S3 in Supporting Information S2) are selected for training the urban neural network (UNN; Section 2.2) and Stage 4 for the TEB to offer the best tradeoff between complexity and accuracy and better model metrics (Figure A1). Overall, TEB's mean bias and mean absolute error improve the more information is provided, notably when the site albedo is given in Stage 3 and 4 (Table S3 in Supporting Information S2). MEM generally has the lowest overall mean bias and mean absolute error for Stage 2.

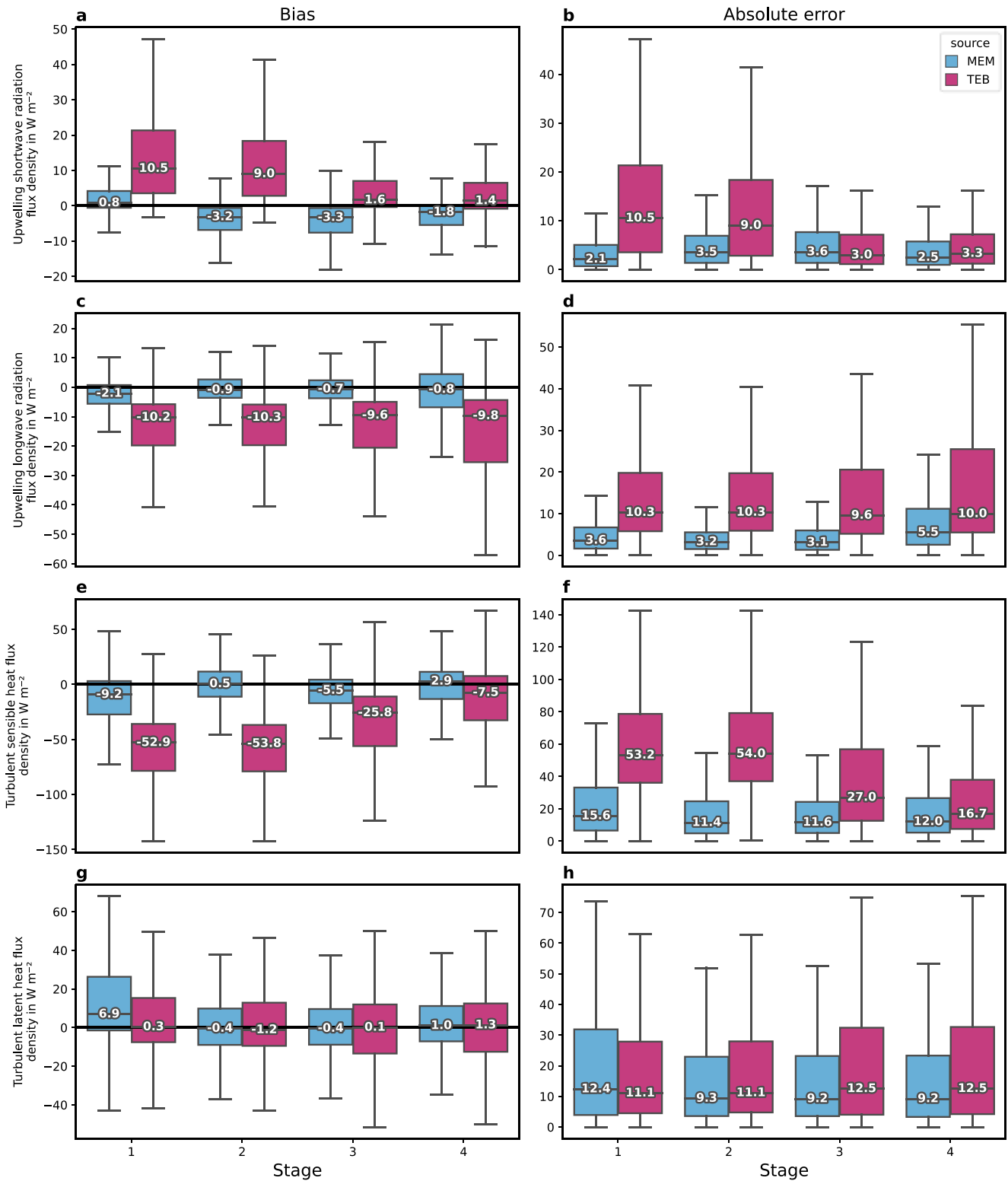


Figure A1. Distribution (boxplot with median (labels) interquartile range (IQR) and whiskers: 1.5 IQR) of the 30-min biases and absolute errors (Section 2.6) relative to observations (OBS) for four Stages (Table S3) of the multi-model ensemble mean (MEM) and Town Energy Balance (TEB) calculated for the test fraction (Section 2.5) of 30-min fluxes of upwelling (a and b) short- and (c and d) longwave radiation, and turbulent (e and f) sensible and (g and h) latent heat.

Data Availability Statement

Software and tools are archived with a Singularity (Kurtzer et al., 2017) image and deposited on Zenodo as described in the scientific reproducibility section of Meyer, Schoetter, Riechert, et al. (2020). Users wishing to download (and reproduce) the results described in this paper can download the data archive at <https://doi.org/10.5281/zenodo.5142960> (Meyer, 2021) and optionally run Singularity on their local or remote systems. Because of licensing restrictions, meteorological forcing (MF), and observational (OBS) and multi-model output (MO) data sets cannot be bundled with the Meyer (2021) data archive and need to be requested separately at <https://doi.org/10.5281/zenodo.4679279> (Grimmond et al., 2021) and at <https://doi.org/10.5281/zenodo.4678387> (Grimmond et al., 2013), respectively.

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