Simulating heat and CO_2 fluxes in Beijing using SUEWS V2020b: Sensitivity to vegetation phenology and maximum conductance

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Abstract. The Surface Urban Energy and Water Balance Scheme (SUEWS) has recently been introduced to include a bottom-up approach to modelling carbon dioxide (CO_2) emissions and ~~sink~~ uptake in urban areas. In this study, SUEWS is evaluated against ~~radiation flux observations and~~ the eddy covariance (EC) measured turbulent fluxes of sensible heat (Q_H), latent heat (Q_E), and CO_2 (F_C) at a densely built neighborhood in Beijing. The model sensitivity to maximum conductance (g_{max}) and leaf area index (LAI) is examined. Site-specific g_{max} is obtained from observations over local vegetation species, and LAI parameters by optimization with remotely sensed LAI obtained from a ~~MODIS/Terra~~ Landsat 7 data product. For the simulation of anthropogenic CO_2 components, local traffic and population data are collected. In the model evaluation, the mismatch between the measurement source area and simulation domain is also considered.

Using the optimized g_{max} and LAI, the modelling of heat fluxes is noticeably improved, showing higher correlation with observations, lower bias, and more realistic seasonal dynamics of Q_E and Q_H. ~~In comparison~~ The effect of the g_{max} adjustment is more significant than the LAI adjustment. Compared to heat fluxes, the F_C module shows lower sensitivity to the ~~choice~~ choices of g_{max} and LAI. This can be explained by the low relative contribution of vegetation to the net F_C in the modelled area. SUEWS successfully reproduces the average diurnal cycle of F_C and annual cumulative sums. Depending on the size of the simulation domain, the modelled annual accumulated F_C ranges from ~~7.2 to 8.5~~ 7.4 to 8.7 kg C m^{-2} yr^{-1}, when compared to 7.5 kg C m^{-2} yr^{-1} observed by EC. Traffic is the dominant CO_2 source, contributing ~~63–73~~59–70% to the annual total CO_2 emissions, followed by human metabolism (14–18%), ~~respiration released~~ building (11–14%), and CO_2 release by vegetation and soil ~~(6–11%)and building heating (6–9%)~~respiration (6–10%). Vegetation photosynthesis offsets only ~~4–8~~5–10% of the total CO_2 emissions. We highlight the importance of choosing the optimal LAI parameters and g_{max} when SUEWS is used to model surface fluxes. The F_C module of SUEWS is a promising tool in quantifying urban CO_2 emissions at the local scale, and therefore assisting to mitigate urban CO_2 emissions.

1 Introduction

Currently, half of the global population resides in urban areas, and this percentage is projected to grow to 68% by the middle of the 21st century (United Nations Department of Economic and Social Affairs, 2019). Urban expansion has reshaped the morphological, thermal, and dynamical properties of the land surface (Grimmond and Oke, 2006; Oke, 1995; Zhu et al., 2016). In addition, intensive human activities in urban areas have caused a large quantity of greenhouse gas emissions (Marcotullio et al., 2013; Velasco and Roth, 2010). Both factors have influenced urban climate from micro to regional scales (Johansson and Emmanuel, 2006; Sarangi et al., 2018; Tan et al., 2010). Climatic and environmental risks due to urbanization are frequently reported, such as heat waves, flooding, and air pollution (Qian et al., 2022; Watts et al., 2015). In this context, there is a pressing need to better understand the effects of urbanization on land-atmosphere interaction, preferably in a quantitative way.

Urban land surface models (ULSMs) are widely used to simulate urban-atmosphere interactions, including the exchanges of energy, water, and CO_2, and hydrological processes (Chen et al., 2011; Masson et al., 2013). The results from the First International Urban Land Surface Model Comparison Project suggested that the most important processes for urban surface energy balance were radiative and vegetation processes (e.g., vegetation fraction, seasonal cycle of vegetation phenology) (Best and Grimm... . Long-term observations with low vegetation cover (<30%) were especially needed to evaluate heat flux simulation, as energy distribution was found sensitive in such environments (Best and Grimmond, 2016).

The Surface Urban Energy and Water balance Scheme (SUEWS) is one of the widely tested ULSMs (Järvi et al., 2011, 2014; Ward et al., 2016). SUEWS is designed to run with surface information (e.g., surface cover fractions) and a minimum amount of model forcing data. In recent years, Supy (SUEWS in Python) was developed to allow Python front-end implementation for broader and easier applications (Sun and Grimmond, 2019). SUEWS has demonstrated good performance against hydrological observations and surface flux observations in several cities in Europe, North America, and Asia (Alexander et al., 2016; Ao et al., 2018; Havu et al., 2022a; Järvi et al., 2011; Ward et al., 2016). In SUEWS, the seasonal cycle of vegetation phenology is indicated by leaf area index (LAI). Previous studies made in two UK cities and Shanghai, China have reported that bias in modelled LAI lead to over- or underestimation in Q_E or Q_H (Ao et al., 2018; Ward et al., 2016). They highlighted the importance of having an appropriate seasonal cycle of LAI in SUEWS. Omidvar et al. (2022) proposed a workflow to derive LAI-related parameters for SUEWS, but it was intended for fully vegetated areas located mainly on the outskirt of cities. Apart from LAI, the maximum conductance (g_{max}) is also critical in scaling the surface conductance (g_s), and therefore the available energy distribution (Ward et al., 2016). However, the impact of LAI-related parameters and g_{max} on the modelled turbulent fluxes has received insufficient attention in urban areas.

Recently, the module of local-scale CO_2 flux (F_C) was incorporated into SUEWS (Järvi et al., 2019). It was found to give reasonable annual sum, seasonal and diurnal cycles against observed F_C in Helsinki, Finland, suggesting that the bottom-up CO_2 emission or uptake estimate in SUEWS can be evaluated by observation-based evidence provided by top-down eddy

covariance (EC) measurements. Furthermore, SUEWS shows the potential for broader use, such as quantifying the carbon sequestration potential of urban vegetation (Havu et al., 2022a), investigating the spatial variability of CO_2 emission, quantifying the contribution of each emission component (Järvi et al., 2019), and therefore assisting urban CO_2 emission mitigation. However, this module has not yet been evaluated in other cities than Helsinki.

Beijing provides a unique test-bed for SUEWS evaluation and application: a mega-city with a population of over 21 million and an increasing urbanized area (MHURD, 2018). The older version of SUEWS (V2017b), has been evaluated and applied in Beijing by Kokkonen et al. (2019), showing good model performance against observed heat fluxes. However, good simulation of turbulent flux does not necessarily imply that the sub-models within give accurate estimates, e.g., LAI and radiative components. Correct presentation of these processes is necessary for more advanced applications such as the prediction of surface exchanges of energy under e.g., future climate scenarios. Besides, the newly-developed F_C module has not yet been evaluated in Beijing.

In this paper, we present a comprehensive evaluation of SUEWS V2020b in simulating surface fluxes of energy and CO_2 in Beijing. The main aims of this study are (1) to evaluate the model performance of SUEWS using different vegetation parameters (default and site-specific) against ~~radiation and~~ the turbulent flux (Q_E, Q_H and F_C) measurements, and (2) to ~~partition F_C into different~~ estimate the anthropogenic and biogenic components~~and quantify the contribution of each component~~' contributions to the F_C with the bottom-up modelling approach by SUEWS. Meanwhile, the impact of the mismatch between the turbulent flux source area and the modelled area is also examined.

2 Model Description

SUEWS is an urban land surface model that simulates the surface energy and water balances, and CO_2 flux at a local (neighborhood) scale ~~(Järvi et al., 2011; Ward et al., 2016; Järvi et al., 2019)~~(Järvi et al., 2011, 2019; Ward et al., 2016). In SUEWS, the modelling domain is separated into seven interacting surface types (buildings, paved surfaces, grass, evergreen trees/shrub, deciduous trees/shrubs, bare soil, and water body), with a single soil layer below each type. SUEWS is designed to run with surface information (e.g., surface cover fractions) and a minimal amount of model forcing data including wind speed (U), relative humidity (RH), air temperature (T_{air}), air pressure (p), precipitation and incoming solar radiation (K_{down}). SUEWS has sub-models for LAI and net all-wave radiation, and users are allowed to modify the parameters of the sub-models based on the information of the modelled domain. In this study, we use SUEWS version V2020b (Havu et al., 2022b).

2.1 Leaf area index model

In SUEWS, leaf growth is accumulated when T_{air} stays above the limit value $T_{base,GDD,i}$ consecutively, denoted by growing-degree-day (GDD). Leaf growth is allowed until GDD reaches the upper boundary $GDD_{full,i}$ or LAI reaches its maximum ($LAI_{max,i}$). Similarly to the leaf growth period, the leaf off period is impacted by $T_{base,SDD,i}$, senescence-degree-day (SDD), and $SDD_{full,i}$ or $LAI_{min,i}$. Leaf fall is controlled by T_{air} or at high latitudes by day length (Järvi et al., 2014). Here, LAI for vegetation type i at the day of year d ($LAI_{d,i}$) is defined as:

$$LAI_{d,i} = \begin{cases} \min\left(LAI_{max,i}, LAI_{d-1,i}^{\omega_1,GDD,i} \cdot GDD_{d,i} \cdot \omega_{2,GDD,i} + LAI_{d-1,i}\right), \text{leaf-on}, T_{base,GDD,i} > T_{d-1} \\ \max\left(LAI_{min,i}, LAI_{d-1,i}^{\omega_1,SDD,i} \cdot SDD_{d,i} \cdot \omega_{2,SDD,i} + LAI_{d-1,i}\right), \text{leaf-off}, T_{d-1} < T_{base,SDD,i}, \end{cases} \tag{1}$$

where $LAI_{max,i}$ and $LAI_{min,i}$ for each vegetation type can be obtained from literature or determined from observations, $\omega_{1/2,GDD/SDD,i}$ represent the growing or senescence rates derived for each study site or use their default values (Järvi et al., 2011; Omidvar et al., 2022), and T_{d-1} is the previous day air temperature mean.

2.2 Radiation fluxes

K_{down} is a required variable in the meteorological forcing data, whereas other radiation components are estimated within SUEWS. Outgoing shortwave radiation (K_{up}) is calculated using a bulk albedo (α) based on the area fraction for each surface type. Incoming longwave radiation (L_{down}) is calculated using T_{air} and RH to estimate the cloud cover and the clear-sky emissivity (Loridan et al., 2011), while outgoing longwave radiation (L_{up}) is estimated by surface emissivity, α, K_{down}, ~~L_{up}~~ L_{down} and T_{air} (Offerle et al., 2003).

2.3 Turbulent heat fluxes

Latent heat flux (Q_E, W m^{-2}) is calculated using the modified Penman-Monteith equation for each surface type:

$$Q_E = \frac{s(Q_N + Q_F - \Delta Q_s) + \rho c_p VPD/r_{av}}{s + \gamma(1 + r_s/r_{av})}, \tag{2}$$

where Q_N (W m^{-2}) is the net all-wave radiation, Q_F (W m^{-2}) the anthropogenic heat flux, ΔQ_S (W m^{-2}) the net storage heat flux, ρ (kg m^{-3}) the air density, c_p (J kg^{-1} K^{-1}) the specific heat capacity of air at constant pressure, VPD (Pa) the vapour pressure deficit, s (Pa °C^{-1}) the slope of the saturation vapour pressure curve, γ (Pa °C^{-1}) the psychrometric constant, r_{av} (s mm^{-1}) the aerodynamic resistance for water vapour, and r_s (s mm^{-1}) the surface resistance. r_s, or its inverse surface conductance g_s (mm s^{-1}), has the form:

$$g_s = \frac{1}{r_s} = \sum_i (g_{max,i} \frac{LAI_i}{LAI_{max,i}} fr_i) G_1 g(K_{down}) g(\Delta q) g(T_{air}) g(\Delta \theta), \tag{3}$$

where $g_{max,i}$ is the maximum conductance of vegetation type i, fr_i is the surface fraction of i, G_1 is a constant connecting stomatal conductance to canopy conductance, $g(K_{down})$, $g(\Delta q)$, $g(T_{air})$, and $g(\Delta \theta)$ are environmental response functions on K_{down}, specific humidity deficit (Δq), air temperature (T_{air}), and soil moisture deficit ($\Delta \theta$), respectively. The functions have the forms (Ward et al., 2016):

$$g(K_{down}) = \frac{K_{down}/(G_2 + K_{down})}{K_{down,max}/(G_2 + K_{down,max})}, \tag{4}$$

$$g(\Delta q) = G_3 + (1 - G_3)G_4^{\Delta q}, \tag{5}$$

$$g(T_{air}) = \frac{(T_{air} - T_L)(T_H - T_{air})^{T_C}}{(G_5 - T_L)(T_H - G_5)^{T_C}}, \tag{6}$$

where

$$T_C = \frac{(T_H - G_5)}{(G_5 - T_L)}, \tag{7}$$

and

$$g(\Delta\theta) = \frac{1 - \exp(G_6(\Delta\theta - \Delta\theta_{WP}))}{1 - \exp(-G_6\Delta\theta_{WP})}. \tag{8}$$

Coefficients $G_2 - G_6$ determine the shape of the curves describing responses of stomatal conductance to each environmental variable. $K_{down,max}$ (W m^{-2}) is the maximum incoming solar radiation, T_L and T_H (°C) are the lower and upper limits for temperature at which photosynthesis and transpiration are off, and $\Delta\theta_{WP}$ (mm) is wilting point deficit. K_{down} (W m^{-2}) is model input, Δq (g kg^{-1}) is calculated from model input RH, T_{air} (°C) is either model input or simulated at 2 m height, and $\Delta\theta$ (mm) is simulated within SUEWS (Järvi et al., 2017). Q_H is determined as the residual from the surface energy balance equation:

$$Q_H = Q_N + Q_F - \Delta Q_{\underline{s}S} - Q_E. \tag{9}$$

2.4 CO$_2$ flux

The F_C module adopts a bottom-up approach to determine the local-scale F_C (μmol m^{-2} s^{-1}), accounting for both anthropogenic ($F_{C,ant}$) and biogenic ($F_{C,bio}$) components (Järvi et al., 2019):

$$F_C \ = \ F_{C,ant} + F_{C,bio} = (F_M + F_V + F_B + F_P) + (F_{pho} + F_{res}) \ . \tag{10}$$

In the Eq. 10, F_M are the CO$_2$ emissions from human metabolism, F_V the emissions from traffic, F_B the emissions from buildings (e.g., combustion of natural gas, coal, and wood), F_P the emissions from local-scale point sources, F_{pho} the CO$_2$ uptake by photosynthesis, and F_{res} ~~vegetation and soil~~ the CO$_2$ release by soil and vegetation respiration. Positive values indicate ~~sources of~~ CO$_2$ emissions and negative values ~~sinks~~ indicate CO$_2$ uptake with respect to the atmosphere. F_{pho} has a negative sign while the rest of the F_C components have a positive sign.

$F_{C,ant}$ relates to the energy balance through Q_F. F_M and F_V are estimated ~~based on~~ with an inventory approach, i.e., based on population density or traffic rate, and their emission factors (EFs). Hourly CO$_2$ emissions from human metabolism on ~~workdays/~~weekdays or weekends ($F_{M,h,d}$, μmol m^{-2} s^{-1}) are calculated using:

$$F_{M,h,d} = p_{h,d} \cdot H_{a,h,d} PP_{h,d} \cdot AP_{h,d} \cdot C_M, \tag{11}$$

where $p_{h,d}$ is the daily average population density (cap ha^{-1}), $H_{a,h,d}$ ~~activity by hourcalculated from the diurnal profiles for population and activity~~ $PP_{h,d}$ the population diurnal profile by hour, $AP_{h,d}$ the activity level diurnal profile by hour, and

C_M the CO_2 ~~released~~ release per person (μmol CO_2 s^{-1} cap^{-1}). The $p_{h,d}$ and $PP_{h,d}$ reconstruct the diurnal population density cycle. $AP_{h,d}$ scales the C_M ~~varies between~~ to vary between the nighttime minimum and daytime maximum values ($C_{M(min,max)}$) to indicate the diurnal cycle of per capita human metabolic intensity.

Hourly traffic CO_2 emissions ($F_{V,h,d}$) on weekdays or weekends are calculated from

$$F_{V,h,d} = \cancel{T_{rd}} Tr_d \cdot E_{c,d} \cdot H_{T,d}, \tag{12}$$

where ~~T_{rd}~~ Tr_d is the mean daily traffic rate within the study area (veh day^{-1} area^{-1}), $H_{T,d}$ the diurnal traffic profiles, and $E_{c,d}$ ~~traffic~~ the traffic the EFs for CO_2 (kg km^{-1} veh^{-1}).

Hourly building CO_2 emissions ($F_{B,h,d}$) on weekdays or weekends are calculated from

$$F_{B,h,d} = [fr_{heat} \cdot (Q_{F,heat} + Q_{F,cool}) + fr_{nonheat} \cdot Q_{F,base} \cdot fr_{QF,base,BEU,d}] \cdot E_{CO2perJ}, \tag{13}$$

where fr_{heat} is the fraction of fossil fuels used for heating, $Q_{F,heat}$ the building heat emission at local scale estimated from the heating-degree-day model (Järvi et al., 2011), $fr_{nonheat}$ the fraction of fossil fuels used for energy other than heating (e.g. ~~combustion from domestic~~ the use of gas stove for cooking), $Q_{F,base}$ the non-temperature related anthropogenic heat flux (W m^{-2}) ~~,~~ including heat emissions from traffic, human metabolism, and electricity usage, $fr_{QF,base,BEU,d}$ the fraction of the $Q_{F,base}$ coming from building energy use on weekdays or weekends, and $E_{CO2perJ}$ the EF for fuels in building energy use (μmol CO_2 J^{-1}). Emissions from single-point sources such as power plants and industrial activities can be included as model inputs.

F_{pho} relates to the energy balance through LAI and the environmental responses of surface conductance (Eq. 3). F_{pho} is calculated using

$$F_{pho} = \sum_i (fr_i F_{pho,max,i} LAI_i) g(T_{air}) g(\Delta q) g(\Delta \theta) g(K_{down}), \tag{14}$$

where $F_{pho,max,i}$ is the maximum photosynthetic rate for vegetation type i.

Soil and vegetation respiration F_{res} (μmol m^{-2} s^{-1}) follows an exponential dependency on T_{air}:

$$F_{res} = \sum_i fr_i \max(a_i \cdot \exp(T_{air} b_i), 0.6), \tag{15}$$

where a_i and b_i are the parameters controlling the temperature dependency, and 0.6 μmol m^{-2} s^{-1} is the minimum respiration in winter time.

3 Study site and measurements

The model domain is ~~located around a 325-m~~ a 1 km circle around the 325 m meteorological tower constructed by Institute of Atmospheric Physics, Chinese Academy of Sciences (IAP tower, 39°58' N, 116°22' E, 60 m above sea level) ~~within~~ located in the 6th Ring area of Beijing, China (Fig. 1 ~~a~~a–d). An EC setup at the height of 47 m on ~~the~~ IAP tower continuously measures

the surface fluxes of Q_E, Q_H and F_C using a 3-dimensional sonic anemometer (Windmaster, Gill, UK) and an open-path

170 infrared gas analyzer (LI-7500A, LI-COR, USA). In addition, all four radiation components are measured at the height of

140 m using a net radiometer (CNR1, Kipp & Zonen, Netherlands). These measurements are used to evaluate SUEWS model

performance. The 1 km radius circle around ~~the~~ IAP tower roughly covers 80% accumulated flux footprint area (Liu et al.,

2012). This area is mainly covered by impervious surfaces (Fig. 1 b). Three patches of urban green spaces are situated to the

east, south, and west to ~~the~~ IAP tower, while the other vegetation is scarcely located along the roads and near the buildings.

175 Most of the impervious surfaces in the source area are residential buildings (Fig. 1 ~~e~~d). A more detailed description of the

surroundings and the used instruments can be found in ~~Liu et al. (2012), Liu et al. (2021) and Cheng et al. (2018)~~the previous

publications by Cheng et al. (2018), Liu et al. (2012), and Liu et al. (2021).
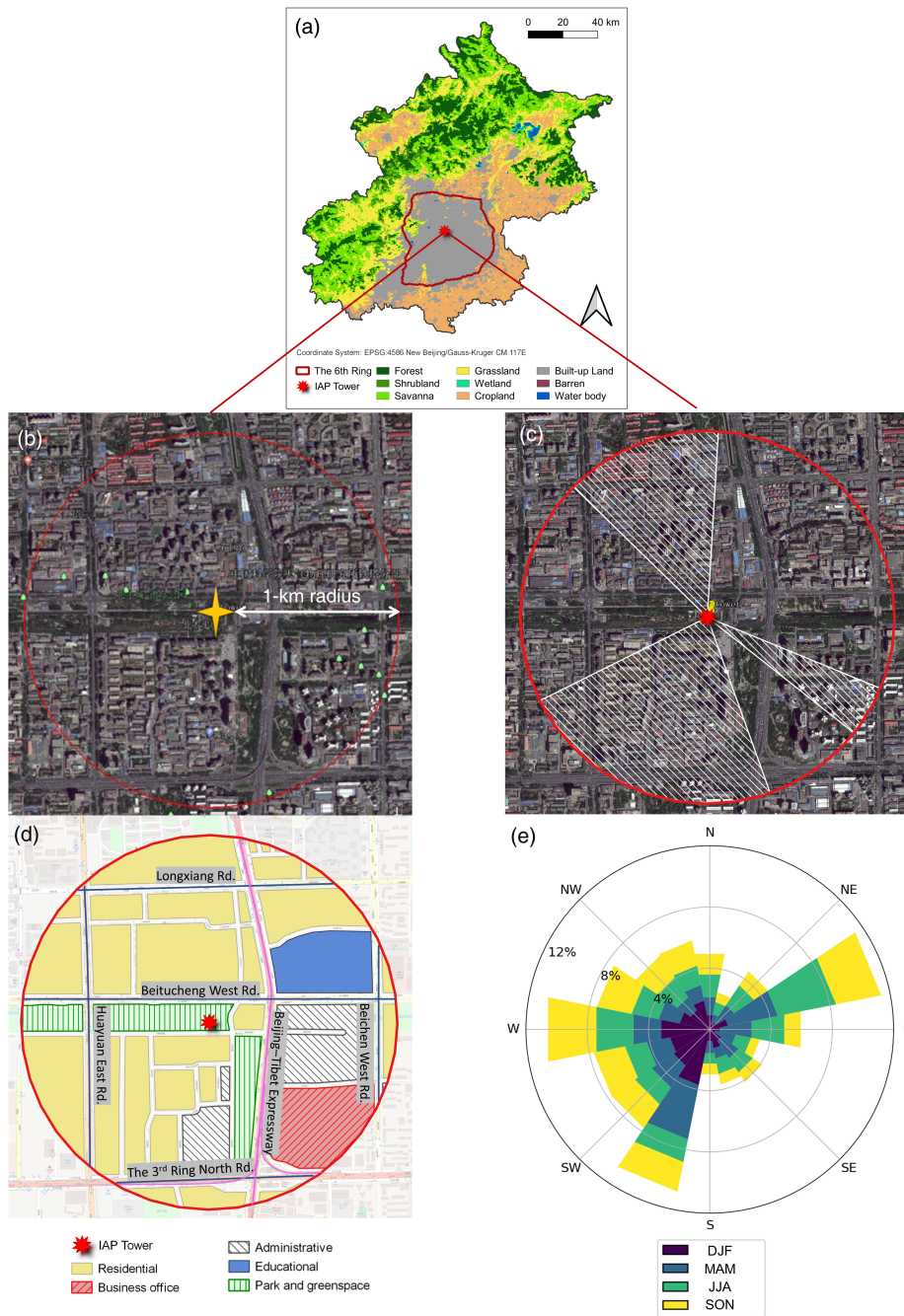
Figure 1. (a) The location of IAP tower and the land cover type within the 6th Ring area of Beijing (~~Terra and Aqua combined Moderate Resolution Imaging Spectroradiometer (~~MODIS ~~)~~ Land Cover Type (MCD12Q1) Version 6, Friedl and Sulla-Menashe (2019))~~(Friedl and Sulla-Menashe, 2019)~~, (b) a satellite image (Google Earth, image ©2022 Maxar Technologies) ~~and~~ over the study area, (c) wind sectors that have been filtered out for data quality control, (d) urban land use categories (EULUC-China) (Gong et al., 2020)~~covering the circle of 1 km radius around the IAP tower~~, and (e) wind direction frequency by season.

The 30-min turbulent flux calculation procedures and the quality controls were described in detail by Cheng et al. (2018). Quality controls such as out-of-limit value removal, spike removal, and a dropout test were conducted on the 10 Hz data during the flux calculation. In order to exclude low-quality data caused by precipitation, dust, or other contamination on the sensor, the records with automatic gain control value $\geq$ 62 were discarded. On top of the procedures by Cheng et al. (2018), the following quality control steps are performed for 30-minute turbulent flux observations in the year 2016. (1) Upper/lower boundary filtering: Q_E observations that fall outside the range from -500 to 1000 W m^{-2}, Q_H from -500 to 1000 W m^{-2}, and F_C from -100 to 200 μmol m^{-2} s^{-1} are removed. (2) Spikes detection: flux values outside 3.5 times of the standard deviation from the 3-day moving mean value are removed (Liu et al., 2012). (3) Wind direction filtering: the wind directions with building heights over 50 m (112–128, 160–243, 314–3°) are removed (Kokkonen et al., 2019) (Fig. 1 c). (4) Stationarity test: data points with stationary indicator > 30% are filtered out (Foken and Wichura, 1996). The percentages of data removed through these 4 steps are 0.2–0.3%, 1.7–2.7%, 37.8–38.2%, and 13.1–17.4%, respectively. The numbers of observations retained after quality control are 8017 for Q_E, 7338 for Q_H, and 7797 for F_C. These 30-minute flux observations are resampled to one–hour resolution. In addition, F_C is gap-filled using seasonal mean diurnal cycle in order to calculate the seasonal and annual sums (Falge et al., 2001).

To optimize the behaviour of LAI with Covariance matric adaptation evolution strategy (CMA-ES)(Appendix A), nine-year Wind directions are mainly from the S-W sectors and the NE-E sectors before the implementation of the wind direction filtering (Fig. 1 e). In winter, wind from the west is more frequently seen than from the east compared to the other seasons. Due to the wind direction filtering, the actual flux source area "seen" by the EC measurement is biased from the 1 km radius circle around IAP tower. The vegetation fraction is 31% in the remaining sectors combined, as compared to 29% in the entire 1 km radius circle (Fig. 1 b–c, Table S1). The model performance in turbulent flux modelling with the land fractions for the remaining sectors is similar to the entire circle (Fig. S1). Therefore, only the results using the land fractions of the entire circle are demonstrated in the main text.

To optimize the behavior of LAI, a six-year time series (2008–2016 2011–2016) of LAI within urban area of Beijing (over an adjacent park near IAP tower is calculated from the atmospherically corrected surface reflectance provided by USGS Landsat 7 Enhanced Thematic Mapper + (ETM+) (30 m spatial resolution) via the Google Earth Engine Data Catalog (Masek et al., 2006). The atmospherically corrected surface reflectance bands have been preprocessed using the scaling factors from the metadata. Next, enhanced vegetation index (EVI) is calculated using the formula (Huete, 1997):

$$EVI = 2.5 \times (NIR - RED) / (NIR + 6 \times RED - 7.5 \times BLUE + 1), \qquad (16)$$

where NIR, RED and BLUE are the 6th Ring area) are derived from the MOD15A2H Version 6 Moderate Resolution Imaging Spectroradiometer (MODIS) combined Leaf Area Index (LAI)and Fraction of Photosynthetically Active Radiation (FPAR)product (Myneni et al., 2015). Related near-infrared, red, and blue bands, respectively. EVI is further used to calculate LAI with the formula (Boegh et al., 2002):

$$LAI = 3.618 \times EVI - 0.118. \qquad (17)$$

The LAI and air temperature time series are subjected to optimization using the Covariance matric adaptation evolution strategy (CMA-ES) (Appendix A). Before the optimization process, values larger than 10 m^2 m^{-2} and negative values are considered as outliers and removed; values during December and January are set to a fixed value, i.e., the average of these months (0.2 m^2 m^{-2}), to reduce the noise in winter and improve the optimization performance. More details can be found at Appendix A. The related data and codes are openly available to reproduce the results (Zheng et al., 2022).

4   Model run

4.1   Forcing meteorological data

The reanalysis dataset WFDE5 (Cucchi et al., 2021) is used as the forcing data for SUEWS. WFDE5 is a bias-corrected dataset of near-surface meteorological variables specifically suited for land surface modelling. It is derived from the fifth generation of the European Centre for Medium-Range Weather Forecasts (ECMWF) atmospheric reanalysis (Hersbach et al., 2020). It is provided at 0.5° spatial and at hourly temporal resolution. WFDE5 is evaluated against observed meteorological observations before it is used as the forcing data for SUEWS (Appendix B).

4.2   Land cover

Land cover types and their fractions needed in the model ~~runs~~ cases are estimated based on aerial images. Paved surface accounts for 46% of the total area, buildings 24%, trees/shrub 13%, grass/lawn 16%, and water 1%. The average building height is 19.1 m (Kokkonen et al., 2019). According to a field survey conducted in the 6th Ring area, the population of deciduous species accounts for 82% of the total number of woody plants investigated (Ma, 2019). Therefore, the surface fraction of deciduous trees is set to 11% and evergreen trees 2%.

4.3   Storage heat flux

To calculate the storage heat flux, Objective Hysteresis Model (OHM) is used (Grimmond and Oke, 1999~~, and the coefficients for~~. The coefficients for all the surface types follow the previous study by Kokkonen et al. (2019). A large portion of the paved surface is asphalt in the study area. Thus, the coefficients are set to the weighted average ~~of case~~ values of asphalt surface (AN99~~to represent the asphalt surface~~) following Ward et al. (2016).

4.4   Human activity

In this study, local parameters of traffic, population dynamics, and building energy use are incorporated ~~when compared to Kokkonen et al. (2019) as~~ in order to estimate Q_F and CO_2 emissions~~are more sensitive to them when compared to anthropogenic heat flux~~.

~~Traffic volume and fleet mix data for each link of~~ The annual mean weekday and weekend diurnal cycle of traffic rate for each road link in 2017 in the study domain ~~for the year 2017 are obtained from Yang et al. (2019). Hourly traffic rate on weekdays or~~

240 ~~weekends~~ are extracted from a dataset based on an extensive road traffic monitoring network (Yang et al., 2019). For weekends and weekdays, the diurnal traffic cycles are calculated independently. The total hourly traffic rate (veh km hour^{-1}) is calculated as the sum of ~~traffic volume weighted by road length within the study domain, and mean~~ the traffic rates, i.e., the product of traffic volume (veh hour^{-1}) and the road link length (km) from all the road links in the study area. The hourly traffic rates are then summed up to the total daily traffic rates ($Tr_{wd/we}$)~~and their diurnal profiles are then obtained (Table 1, Fig. 2)~~.

245 ~~The average traffic CO$_2$ EFs are calculated using the method following Zhang et al. (2018) based on the self-reported fuel records, on-road measurements, vehicle category and speed obtained in Beijing (Zhang et al., 2014; Wen et al., 2020, 2022)~~ veh km^{-1} day^{-1})~~,~~ and divided by the total modelling area, yielding Tr_d. Finally, the diurnal traffic profiles ($H_{T,d}$) are obtained by normalizing the diurnal cycles of the total hourly traffic rate (Table 1~~). Traffic rate during daytime is higher than in the nighttime, and it is higher on weekdays than on weekends throughout the day (~~, Fig. 2).

250 Annual average diurnal cycle of population density within the model domain is obtained from a dataset of hourly population dynamics at 500-m resolution generated from remotely sensed and geospatial data over the years 2015 and 2016 (Zhao et al., 2021) (Fig. 2). As there are several residential building areas located within the model domain (Fig. 1 ~~e~~d), population density increases in the evening when residents get home from work, remains high throughout the night, and decreases in the morning. Weekdays and weekends share the same diurnal cycle of population density in our study.

255 Heating in Beijing is dominated by central heating, supplied mainly at the district level. The sources include cogeneration plants fueled by coal or gas, and district boilers powered by coal, oil, or gas. ~~In 2015, the ratio of district boilers heating capacity to cogeneration plants was 4.2:1 (Zhang et al., 2019).~~ Cogeneration plants are usually located at ~~sub-urban~~ suburban or rural areas, and there are no cogeneration plants within the model domain, so their contribution to CO$_2$ emission is neglected in this study. In comparison, boiler plants are very common: over 5000 coal-fired and 1000 gas-fired heating boilers are located

260 surrounding the populated areas in 2014 (Cui et al., 2019). ~~The exact number or heating capacity is unknown in the study area, but three boiler plants are seen within 2~~ We investigated the boiler plants near IAP tower through interviews and found that there were at least 11 of them located at multiple directions within 1.5 km distance from ~~the IAP tower~~through Baidu Map. ~~Their~~ IAP tower. For the known boiler plants, 8 of them have a chimney height lower than 20 m. Thus, their CO$_2$ emissions are very likely to be observed by EC ~~during~~ at 47 m during the heating season. ~~Therefore, fraction of fossil fuels used for heating~~

265 ~~(Fr_{heat}) is set to 0.81 based on the ratio of heating capacity.~~ Unfortunately, the heating capacity and detailed information regarding the fuel combustion for each boiler plant are unknown or restricted from access. Therefore, it is challenging to treat the boiler CO$_2$ emissions as point sources. As an alternative, SUEWS first estimates the anthropogenic heat ~~,~~release from heating $Q_{F,heat}$ and then converts the heat into local CO$_2$ ~~combustion~~ release using the EF and ~~emission fractions.~~ the fraction of fossil fuels used for heating fr_{heat} (Eq. 13).

270 In 2015, the ratio of district boilers heating capacity to cogeneration plants was 4.2:1 (Zhang et al., 2019). Correspondingly, fr_{heat} is set to 0.81 to represent the heating capacity from local boiler plants. The value of natural gas consumption over the annual total heating supply is 3.2×10^6 ton coal equivalent (tce) and the value for coal consumption 2.6×10^6 tce in 2015. The consumption of the rest of the fuel types is only 3.8×10^5 tce (MHURD, 2018). The EFs of heating supply are 96.51 Tg CO$_2$/10^{19} J for coal-fired boiler, and 56.17 Tg CO$_2$/10^{19}J for gas-fired boiler, respectively (Du et al., 2018). Therefore,

the EF for fuels used in building energy use ($E_{CO2perJ}$) in SUEWS takes the average of the EFs of natural gas and coal weighted by their annual consumption, i.e., 0.1688 μmol CO_2 J^{-1} (Table 1). In addition, SUEWS needs a temperature limit (base temperature, T_{base_HC}) to indicate when heating takes place in the heating-degree-day model. Central heating usually starts around 15th of November and lasts until 15th of March, when the outdoor air temperature is around 12 °C. Therefore, this value is given to SUEWS T_{base_HC} to replace the default value (18.2 °C) (Järvi et al., 2011).

~~Household fuel combustion, mainly from cooking, takes place throughout the year, but its CO_2 emission are relatively small. An observational study shows that CO_2 emitted from fuel combustion in household cooking contributes only 6% of the indoor CO_2, and this percentage is low, compared with contribution by human metabolism (30%) (Shen et al.~~ Statistics showed that urban household living consumed liquefied petroleum gas 27.9×10^7 kg of coal equivalent (kgce), gas 17.1×10^8 kgce, and electricity 20.46×10^8 in 2016 (BMBS, 2017), indicating that 50% of the household energy use involved on-site CO2 emissions. Therefore, ~~2020). Therefore, we set 20% to~~ the non-heating ~~energy fraction ($Fr_{nonheat}$)~~ fraction ($fr_{nonheat}$) is set to 0.5.

Table 1. Parameters related to anthropogenic heat and CO_2 emissions.

Parameter	Notation	Value	Reference
$C_{M(min)}$	Minimum CO_2 release per capita	120 μmol CO_2 s^{-1} cap^{-1}	Ward et al. (2013)
$C_{M(max)}$	Maximum CO_2 release per capita	280 μmol CO_2 s^{-1} cap^{-1}	Moriwaki and Kanda (2004)
$E_{c,wd}$	Traffic CO_2 EF for weekday	0.207 kg km^{-1} veh^{-1} (4.70×10^6 μmol CO_2 veh^{-1} km^{-1})	~~Zhang et al. (2014); Wen et al. (2020, 20~~
$E_{c,we}$	Traffic CO_2 EF for weekend	0.209 kg km^{-1} veh^{-1} (4.75×10^6 μmol CO_2 veh^{-1} km^{-1})	~~Zhang et al. (2014); Wen et al. (2020, 20~~
Tr_{wd}	Mean daily traffic rate for weekday	0.3260 veh km day^{-1} m^{-2}	Yang et al. (2019)
Tr_{we}	Mean daily traffic rate for weekend	0.2664 veh km day^{-1} m^{-2}	Yang et al. (2019)
Fr_{heat}	Fraction of fossil fuels used for heating	0.81	~~Cui et al. (2019); Zhang et al. (2019)~~Cu ~~MHURD (2018)~~Zhang et al. (2019)
$Fr_{nonheat}$	Fraction of fossil fuels used for energy	~~0.2~~0.5	~~this study~~ BMBS, 2017
$E_{CO2perJ}$	EF for fuels used in building energy use	0.1688 μmol CO_2 J^{-1}	Cui et al. (2019)
T_{base_HC}	Base temperature for heating degree day	12 °C	this study
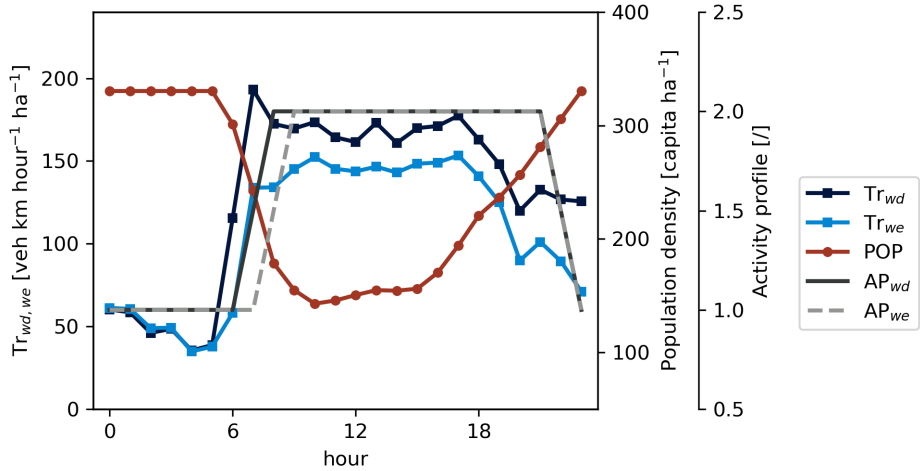
Figure 2. Annual average diurnal cycle of traffic rate ~~(vehicle kilometers travelled, VKT)~~ for weekday (~~VKT_WD~~Tr_{wd}) ~~,~~and weekend (~~VKT_WE~~Tr_{we}), ~~and~~ population density (POP), and the activity profiles for weekday (AP_{wd}) and weekend (AP_{we}) within the 1 km radius circle around ~~the~~ IAP tower.

4.5 Evaluation design

Two different groups of SUEWS runs are made around ~~the~~ IAP tower (Fig. 1c). The first run over the years 2009 to 2011 is to evaluate the modelled radiation components against observations. The first 16 months are the spin-up period, and the actual
290 model evaluation ~~are~~ is made from May 2010 to June 2011, when the radiation observations are available. The second SUEWS run from 2015–2016 is to evaluate the turbulent fluxes. The first year is used as a spin-up period and only the year 2016 is used in the evaluation.

The model performance of radiation fluxes is evaluated prior to the simulation of turbulent heat fluxes. The results show that SUEWS is applicable to provide realistic estimates of radiation fluxes in the study area despite the absence of site-specific
295 parameters (Appendix C). The calculation of radiation fluxes is mostly dependent on the land cover fractions under the current scheme adopted by SUEWS (Loridan et al., 2011; Offerle et al., 2003). No visible change in land use type is observed according to satellite images from Google Earth within the modelled area between 2010 and 2016 (figure not shown). Therefore, we assume that the evaluation of radiation fluxes using observations in the years 2011–2012 holds true in 2016.

4.5.1 Sensitivity to vegetation-related parameters

300 In order to test the model's sensitivity of radiation and turbulent fluxes to vegetation-related parameters, four model ~~runs~~ cases are designed as follows:

1. Case **base**: control run where model parameters are considered "default" following Kokkonen et al. (2019) (Table ~~S1–S3~~S2–S4). The exceptions are: (1) parameters in the environmental response functions (Eq.4 –7) of surface conductance which follow those by Havu et al. (2022a) (Table 2), because the product of response functions calculated

305   following Kokkonen et al. (2019) is too low (95th percentile = 0.19) to obtain realistic estimate of photosynthetic rate; (2) biogenic parameters for Eq.14–15 and soil properties which were updated following Havu et al. (2022a) (Table 2). In addition, $F_{pho,max}$ for grass/lawn (5.5 μmol m^{-2} s^{-1}) is obtained from EC observations of CO_2 flux made over urban lawn in Helsinki in summer 2021 by fitting the conductance parameters ($F_{pho,max,grass}$, $G_2 - G_6$) to the observations following Järvi et al. (2019) (Appendix D).

310   2. Case **LAI**: Same as ~~the~~ case **base** but the parameters for Eq.1 describing the annual behaviour of LAI are optimized using remotely-sensed LAI and CMA-ES (Appendix A). The new optimized LAI parameters are compared with case **base** in Table 3.

   3. Case **gs**: Same as ~~the~~ case **base** but with g_{max} values collected from observational studies over vegetation species in Beijing (Appendix E). The site-specific g_{max} are in general lower than the values used by case **base** (Table 4).

315   4. Case **gs_LAI**: Same as ~~the~~ case **base**, but with both LAI and g_{max} modified as described in case **LAI** and case **gs**.

Table 2. SUEWS biogenic model parameters used for all case runs in this study.

Parameter	Evergreen/deciduous tree	Grass/lawn	Reference
$\text{LAI}_{i,max}$ ($m^2\ m^{-2}$)	5.1[a]/5.5[b]	5.9	Järvi et al. (2011)
$\text{LAI}_{i,min}$ ($m^2\ m^{-2}$)	4.0[a]/1.0[b]	1.6	Järvi et al. (2011)
$F_{pho,max,i}$ ($\mu mol\ m^{-2}\ s^{-1}$)	8.4[c]	5.5[d]	[c]Havu et al. (2022a); [d]this study
G_1	3.5	3.5	Havu et al. (2022a)
G_2	477	477	Havu et al. (2022a)
G_3	0.66	0.66	Havu et al. (2022a)
G_4	0.89	0.89	Havu et al. (2022a)
G_5	30	30	Havu et al. (2022a)
G_6	0.36	0.36	Havu et al. (2022a)
$\Delta\theta_{WP}$ (mm)	132	132	Havu et al. (2022a)
$K_{down,max}$ ($W\ m^{-2}$)	1200	1200	Järvi et al. (2014)
T_L (°C)	-10	-10	Ward et al. (2016)
T_H (°C)	55	55	Ward et al. (2016)
a_i	0.78[c]	2.1[e]	[c]Havu et al. (2022a); [e]Järvi et al. (2019)
b_i	0.08[c]	0.06[e]	[c]Havu et al. (2022a); [e]Järvi et al. (2019)
Soil depth (mm)	1000[c]	349[f]	[c]Havu et al. (2022a); [f]Kokkonen et al. (2019)

[a] Evergreen tree

[b] Deciduous tree

Comparison of maximum conductances (g_{max}) between the case **base** and case **gs/gs_LAI**. Parameters for case **base** follow Järvi et al. (2011). More details can be found in Appendix E. case **base** case **gs/gs_LAI**Evergreen tree 7.4 1.4 Deciduous tree 11.7 7.0 Grass 40.0 3.7

Table 3. Comparison in leaf area index (LAI) parameters between case **base** and case **LAI/gs_LAI**. All vegetation types (evergreen tree, deciduous tree and grass) use the same LAI parameters within one case. Case **base** values are as in Järvi et al. (2011).

	LAI parameters	
	case **base**	case **LAI/gs_LAI**
$T_{base,GDD}$ (°C)	5	~~3.8~~ 5.7
$T_{base,SDD}$ (°C)	10	~~35~~ 22
GDD_{full} (°C)	300	~~2235~~ 446
SDD_{full} (°C)	-450	~~-2365~~ -1000
$\omega_{1,GDD}$	0.04	~~-1.85~~ -1.42
$\omega_{2,GDD}$	0.001	~~0.00029~~ 0.00258
$\omega_{1,SDD}$	-1.5	~~1.28~~ 2.0
$\omega_{2,SDD}$	0.0015	~~0.000025~~ 0.0001

Table 4. Comparison of maximum conductances (g_{max}) between case **base** and case **gs/gs_LAI**. Parameters for case **base** follow Järvi et al. (2011). More details can be found in Appendix E.

	g_{max} (mm s^{-1})	
	case **base**	case **gs/gs_LAI**
Evergreen tree	7.4	1.4
Deciduous tree	11.7	7.0
Grass	40.0	3.7

4.5.2 Sensitivity to radius of modelled area

320 SUEWS output will be evaluated against ~~EC measured~~ EC-measured turbulent fluxes, but the challenge is that the source area of the observations are different to the exact modelling domain. To consider the impact of the chosen modelling domain on model evaluation, we designed three additional model ~~runs~~ cases where different radius circular areas around ~~the~~ IAP tower are considered. The default run is with the 1 km radius circle, but ~~we also run SUEWS~~ SUEWS is also run within 500 m, 750 m, and 1500 m circular areas, corresponding to the flux footprint of roughly 60%, 70%, and 80–90%, respectively (Liu et al.,
325 2012). Used vegetation parameters are as in case **gs_LAI**, but land surface fractions, population, and traffic parameters are modified accordingly (Appendix F).

4.6 Statistical metrics for model evaluation

Common statistical metrics are used to quantify the model performance, including, coefficient of determination (R^2), root-mean-square error (RMSE) and mean bias error (MBE). Simple linear regression is used to estimate the relationship between the model output and the observations, and the square of the correlation coefficient is taken as R^2. The other statistical metrics are defined as follows:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}}, \text{and} \tag{18}$$

$$\text{MBE} = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i), \tag{19}$$

where $\hat{y}_i$ is the modelled and y_i the measured value. Statistical metrics are calculated at annual and seasonal scale, i.e., DJF (winter), MAM (spring), JJA (summer), SON (autumn).

5 Results and Discussion

5.1 Seasonal dynamics of the optimized LAI

The control case **base** simulates the onset of leaf growth and the ending of senescence reasonably well (Fig. 3). The performance of LAI modelling is further improved after the optimization (Appendix A). In case **base**, the modelled LAI starts to increase rapidly from day of year (DOY) 70 and plateaus at DOY 105, which is too early when compared to the remotely sensed LAI (Landsat 7 LAI). The optimized LAI starts to grow at the same time but slightly slower and peaks 20 days later than **base**. In autumn, LAI modelled by case base drops rapidly at DOY 310, while the optimized LAI starts to decline rapidly at DOY 267. LAI model with the optimized parameters is better at capturing the behavior of senescence than in the control case **base**.

Although previous studies suggested that LAI was generally modelled well using default parameters following Järvi et al. (2011), Ward et al. (2016) reported that leaf-on is reached too early and suddenly in spring in two UK cities. On the contrary, Ao et al. (2018) showed that the simulated LAI might be lower than reality when vegetation remained green in winter and spring in Shanghai, China. These lead to the bias in g_s and therefore Q_E estimates (Eq. 2–3). In Beijing, the rainy season lasts from May to October, while the other time of the year is the dry season (Liu et al., 2012). It is possible that the distinct dry season leads to a lack of soil moisture in spring and autumn and thus influences the LAI seasonal dynamics if there is no external water input (Omidvar et al., 2022). However, the urban green spaces in Beijing are usually sufficiently or even excessively irrigated (Zhang et al., 2017). Observations also provided evidence to support the relationship between air temperature and phenological

dynamics in the urban environment in Beijing (Lu et al., 2006; Luo et al., 2007). Therefore, the air temperature-dependent LAI model is applicable in Beijing, but the "default" LAI parameters might be not suitable. We recommend evaluating the LAI model when SUEWS is applied to a different city, and deriving the optimal LAI parameters if necessary.

Input or modelled vs. observed hourly radiation fluxes, including (a–d) incoming solar radiation (K_{down}), (e–h) outgoing shortwave radiation (K_{up}), (i–l) incoming longwave radiation (L_{up}), (m–p) outgoing longwave radiation (L_{up}), and (q–t) net radiation (Q_N) from May 2010 to June 2011. Note that only K_{down} is input and the rest are model output.
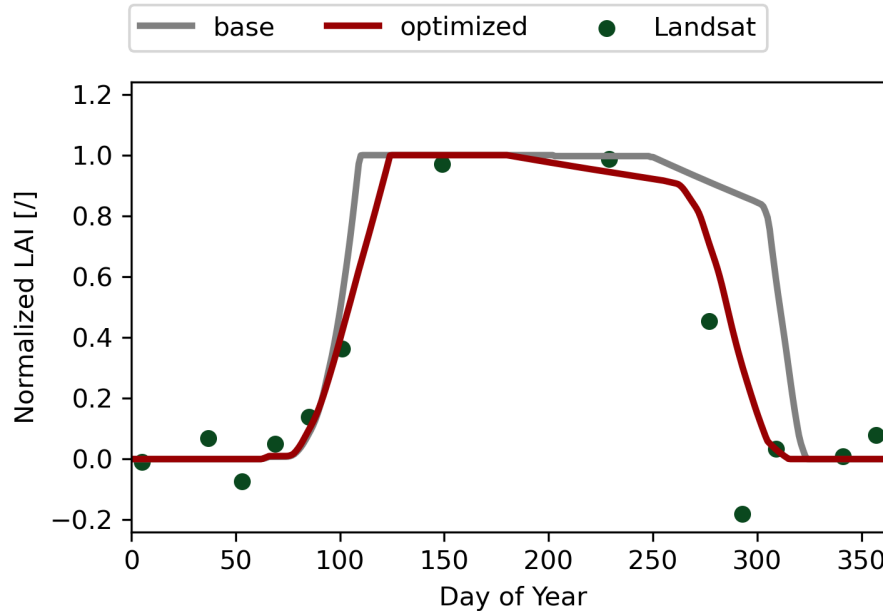
Figure 3. Normalized LAI in 2016, where the value 0 (1) represents the minimum (maximum) of LAI. "Base" denotes the modelled LAI for case **base**, "Landsat" the remotely sensed LAI of the adjacent park near IAP tower, and "optimized" the modelled LAI using the parameters derived with CMA-ES (Appendix A).

360 **5.2 Evaluation of radiation fluxes**

Four model experiments are conducted to examine the impact of g_{max} and LAI seasonal dynamics on the modelled radiation fluxes (See Sect. 4.5.1). However, the choice of g_{max} and LAI parameters has only a minor impact on the modelled radiation fluxes (K_{down}, K_{up}, L_{down}, L_{up}). For all of them, the R^2 between the case **gs_LAI** and the other cases is 1, and the absolute values of RMSE and MBE are lower than 0.002 W m^{-2} and 10^{-4} W m^{-2}, respectively. Therefore, only the case **gs_LAI** is
365 further analyzed in this section.

The model performance of SUEWS in simulating radiation fluxes is good (Fig. C1, Table C1) and it can reproduce the diurnal cycle of each radiation flux well (Fig. C2). K_{up} is overestimated in all seasons with MBE ranging from 0 to 10 W m^{-2}. At least partly, this overestimation can be explained by the positive bias (MBE > 15 W m^{-2} in all seasons) of WFDE5

K_{down} when compared to the observed K_{down} (Appendix B). The overestimation in K_{up} can also be caused by surface albedo. Observational studies have shown that the urban surface albedo near the IAP tower varies between 0.1 and 0.15 with season (Jiang et al., 2007; Miao et al., 2012). The annual average albedo for modelling domain given to SUEWS is 0.14, which is relatively high but still consistent with the observations. Larger positive bias is observed in summer than in winter. In SUEWS, albedo is allowed to vary between summer and winter if specified, and this can help to lower the bias in summer when the albedo for vegetation is low, but this is likely to have only a minor impact because the vegetated fraction is low.

Average diurnal cycle of input or modelled and observed hourly radiation fluxes by season, including (a–d) incoming solar radiation (K_{down}), (e–h) outgoing shortwave radiation (K_{up}), (i–l) incoming longwave radiation (L_{up}), (m–p) outgoing longwave radiation (L_{up}), and (q–t) net radiation (Q_N) from May 2010 to June 2011. Shading area denotes the standard deviation. Note that only K_{down} is input and the rest are model output.

The average seasonal and diurnal cycles of L_{down} are well captured by the model (Fig. C1 i–l), although R^2 (0.68–0.88) is lower than with other radiation fluxes. The difference might result from the discrepancy between the observed and modelled cloud fraction as clear skies and overcast conditions are especially difficult to capture by the radiation model NARP, as reported also by Ao et al. (2016) and Ward et al. (2016). The diurnal amplitude of L_{up} is slightly overestimated by SUEWS (Fig. C2 m–p). The model tends to overestimate L_{up} particularly at high values of L_{up} (Fig. C1 m–p). The values of emissivity of building materials used in SUEWS might be slightly lower than in reality.

We conclude that SUEWS is applicable to provide realistic estimate of radiation fluxes in Beijing, in general accordance with previous studies (Järvi et al., 2014; Karsisto et al., 2016; Ward et al., 2016), despite the absence of site-specific parameters.

SUEWS model performance statistics for radiation fluxes. The abbreviations are the same as Fig. C1. Note that K_{down} is an input and others are output of SUEWS. Season R^2 RMSE MBE N *K_{down}DJF 0.94 52.3 19.5 2160 MAM 0.93 82.6 19.8 2940 JJA 0.86 110.4 39.3 2728 SON 0.93 59.6 16.6 2150 *K_{up}DJF 0.88 9.2 0.2 2160 MAM 0.92 14.8 5.0 2940 JJA 0.88 18.0 8.1 2728 SON 0.91 11.6 3.3 2150 *L_{down}DJF 0.74 16.0 -2.4 2160 MAM 0.86 20.5 -10.0 2940 JJA 0.68 18.1 8.8 2728 SON 0.88 23.7 12.9 2150 *L_{up}DJF 0.80 15.3 3.8 2160 MAM 0.90 18.6 3.2 2940 JJA 0.79 22.1 10.5 2728 SON 0.91 18.6 9.2 2150 *Q_NDJF 0.94 38.0 13.2 2160 MAM 0.93 64.6 1.5 2940 JJA 0.86 87.0 29.5 2728 SON 0.92 50.8 17.0 2150

5.2 Evaluation of turbulent heat fluxes modelling

Both observed Q_E and Q_H reach their maxima around noon (Fig. 4). The observed Q_E has the largest amplitude during the summer months~~(JJA)~~, while Q_H during the spring months~~(MAM)~~. All four model ~~runs~~ cases capture their diurnal cycles, but large differences in the amplitude and model performance are observed among the model ~~runs~~ cases (Fig. 5).

In ~~the~~ case **base**, the model overestimates Q_E (with MBE from -7.4 to 48.6 W m^{-2}) except in winter months (~~DJF) (~~Fig. 5). With the optimized LAI (case **LAI**), ~~slightly better~~ model performance in Q_E ~~is seen with lower RMSE (11.5–91.2~~ remains virtually unchanged, with RMSE (12.1–94.1 W m^{-2}) and ~~larger~~ R^2 (~~0.20~~0.17–~~0.58~~0.53) when compared to case **base** (with RMSE 11.7–96.1 W m^{-2} and R^2 0.20~~–0.51) .~~–0.51) (Fig. 5 a–c). Q_E is to a large extent determined by surface conductance which ~~for the modelled area~~ is scaled by g_{max} of each vegetated surface for the modelled area (Eq. 3). Clear improvement is observed when the local g_{max} is used (case **gs**), especially during summer~~, when the~~. The overestimation of Q_E is largely reduced, RMSE drops to 11.3–54.7 W m^{-2}, and R^2 increases to 0.25–0.61. ~~The introduction of local g_{max} improves the model performance more than the optimized LAI. With both~~ With both the optimized LAI and the local g_{max} introduced (case **gs_LAI**), the R^2 ~~and RMSE are similar to those at~~ is similar to case **gs**, while ~~MBE drops below 0 in each season, indicating the~~ RMSE slightly decreases by 1–2 W m^{-2} in spring and summer compared to case **gs**. Q_E is ~~slightly~~ underestimated throughout the ~~year. The underestimation can be explained by the missing of combustion-derived water vapor in SUEWS as observational day in winter (MBE = -8.3 W m^{-2}).~~ Observational studies have shown that combustion-derived water vapor often contributes 5–10% of total urban humidity during heating season (Fiorella et al., 2018; Liu et al., 2022; Salmon et al., 2017). The observed Q_E ranges from 0 to 30 W m^{-2} in winter when vegetation is dormant; this suggests that combustion and evaporation, as the dominant sources of Q_E, might lead to Q_E at this magnitude. The anthropogenic water vapor release might be underestimated by SUEWS in winter.
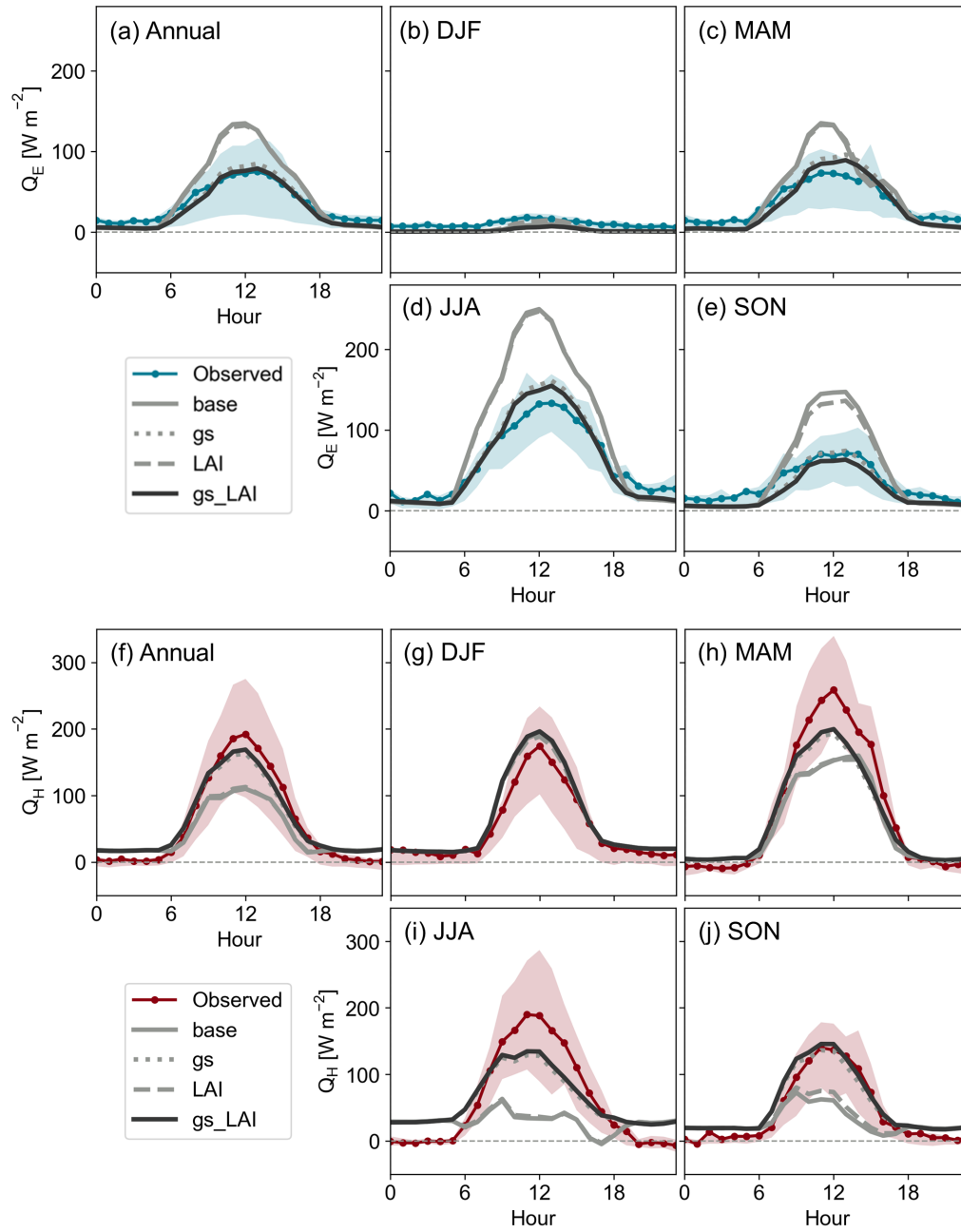
Figure 4. Annual and seasonal mean diurnal cycles of observed and modelled (a–e) latent heat flux (Q_E) and (f–j) sensible heat flux (Q_H) for the four model ~~runs~~ cases (case **base**, **gs**, **LAI**, and **gs_LAI**) in the year 2016. The shaded area denotes the interquartile range.
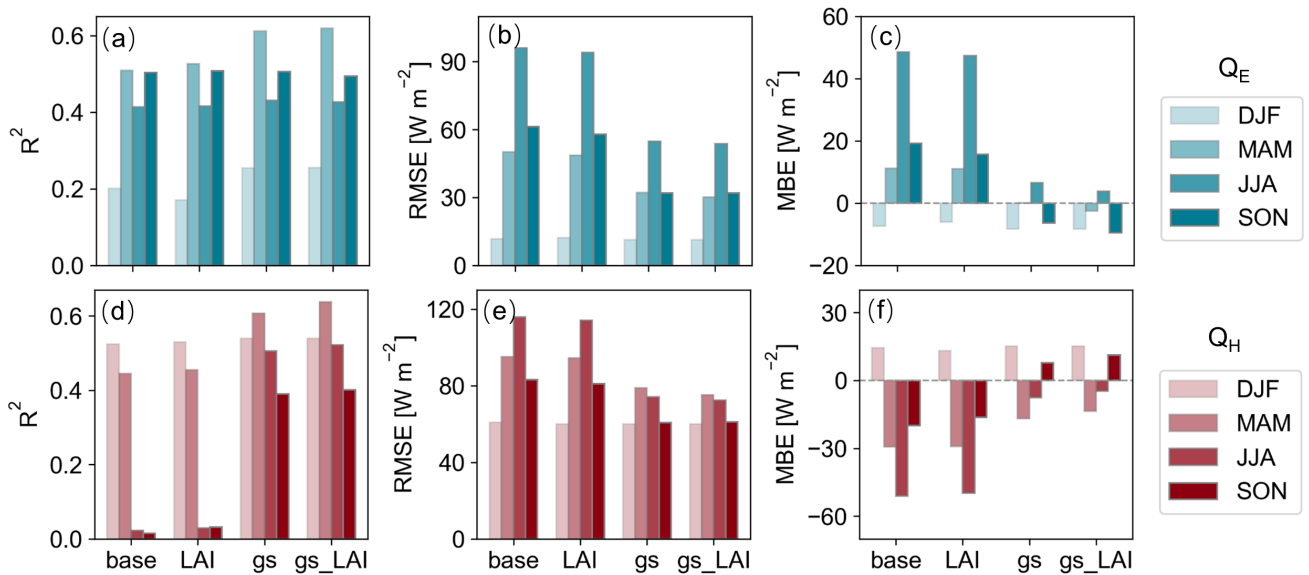
Figure 5. Model performance statistics R^2, RMSE and MBE of (a–c) latent heat flux (Q_E) and (d–f) sensible heat flux (Q_H) for the four model ~~runs~~ cases (case **base**, **gs**, **LAI**, and **gs_LAI**) in the year 2016.

In SUEWS, Q_H is estimated as the residual of energy balance, and is therefore directly affected by the modelled Q_E. As a result of overestimating Q_E in case **base**, Q_H is greatly underestimated with MBE -51.1–14.4 W m^{-2} and RMSE 60.9–116.0 W m^{-2}. R^2 in summer months and autumn months ~~(SON)~~ are lower than 0.1. The model performance is barely improved by the optimized LAI (case **LAI**) ~~, but~~ but it is noticeably improved after the local g_{max} is introduced (case **gs**) (Fig. 5 d–f). The best model performance for Q_H is obtained by case **gs_LAI**, decreasing the magnitudes of MBE to ~~-7.6–8.9~~ -13.6–15.2 W m^{-2} and RMSE to ~~58.0–69.1~~ 60.1–75.3 W m^{-2}, and increasing R^2 to ~~0.42–0.72~~ 0.40–0.64 (Fig. 5 d–e).

Q_H is also influenced by Q_F. Nighttime Q_F in summer might be overestimated, leading to the overestimation in Q_H. Turbulent heat fluxes are also related to ΔQ_S. Both Q_E and Q_H correlate with ΔQs negatively (Eq. 2, Eq. 9). For instance, Q_E is underestimated while Q_H is overestimated at noon in summer in case **gs_LAI**. The decrease in ΔQ_S will lead to a simultaneous increase in Q_E and Q_H, lowering Q_H's bias while increasing Q_E's. Therefore, the adjustment of ΔQ_S can hardly improve the Q_E and Q_H modelling at the same time.

Our results suggest that ~~both altering the values of~~ the model performance of heat fluxes is more sensitive to the adjustment of g_{max} ~~based on observations and LAI model optimization can serve as effective approaches to improving heat fluxes modelling~~ than to the change of LAI seasonal dynamics. By incorporating local LAI and g_{max}, SUEWS simulates the heat fluxes noticeably better, increasing R^2 by 0.03 (0.30) and decreasing RMSE by 27.0 (23.7) W m^{-2} for Q_E (Q_H) compared to case **base**.

5.3 Evaluation of CO$_2$ fluxes modelling

5.3.1 Model performance

SUEWS ~~basically~~ reproduces the average annual and seasonal diurnal cycle of observed F_C (Fig. 6). The diurnal behaviour is dominated by on-road traffic emission, which reaches 22.6 and 23.0 μmol m^{-2} s^{-1} for the morning peak and afternoon peak, respectively, during the rush hours (Fig. 7). Human metabolism (maximum 4.8 μmol m^{-2} s^{-1}) is the second largest source of CO$_2$ emissions. In winter, the building CO$_2$ emission has a maximum of ~~5.3~~ 6.7 μmol m^{-2} s^{-1} in the daytime. The maximum photosynthesis rate is ~~5.0~~ 5.9 μmol m^{-2} s^{-1} around noon in summer, while soil and vegetation respiration constantly serves as a CO$_2$ source with a rate lower than 3.6 μmol m^{-2} s^{-1}.

Each of the model performance statistics of F_C is of a similar magnitude among cases, indicating the F_C modelling is far less sensitive to the ~~choice~~ choices of g_{max} and LAI-related parameters than Q_E and Q_H shown in Sect. 5.2 (Fig. 8). Under the current parameterizations, F_{res} considers only air temperature (Eq. 15). The adjustments of g_{max} and LAI parameters affect the modelled heat fluxes, influencing 2 m air temperature, and finally F_{res}, but the difference in annual CO$_2$ release from respiration is less than 0.01 kg C m^{-2} yr^{-1} among cases. F_{pho} is sensitive to the adjustments of g_{max} and LAI parameters. In case **base**, the large values of g_{max} allow relatively high evapotranspiration (namely Q_E). As a result, the average $\Delta\theta$ during January and June is larger than 105 mm, which is only 27 mm lower than the wilting point deficit ($\Delta\theta_{WP}$). The dry soil lowers the surface conductance and photosynthetic CO$_2$ uptake through the limiting function of $g(\Delta\theta)$ (Eq. 8). As the local g_{max} is introduced, the soil remains moister with $\Delta\theta$ lower than 75 mm throughout the year, allowing a more favourable condition for the photosynthetic CO$_2$ assimilation. The CO$_2$ assimilated through photosynthesis is 0.57 kg C m^{-2} yr^{-1} in case **gs**, which is 0.21 kg C m^{-2} yr^{-1} higher than in case base. The LAI reduction in spring and autumn in case **gs_LAI**, on the other hand, directly limits surface conductance and photosynthesis (Eq. 14), leading to a decrease by 0.07 kg C m^{-2} yr^{-1} in annual photosynthetic CO$_2$ uptake when compared to case **gs**.

In SUEWS, photosynthetic ~~rate and respiration are multiplied by the percentages~~ and respiration rates are proportional to the fractions of vegetated surfaces, which account for only 29% of the modelled area. The magnitude of ~~photosynthetic rate~~ F_{pho} is substantially lower than the traffic emission, making the effect of photosynthesis, as well as its response to the adjustments of g_{max} and LAI parameters, hardly visible in ~~F_C diurnal cycle~~ the F_C diurnal cycles.

Expectedly, SUEWS has difficulty in capturing the hourly variability of F_C, resulting in the overall low R^2 (0.16–0.~~21~~22) and high RMSE (~~12.6~~ 12.9–16.4 μmol m^{-2} s^{-1}) (Fig. 8 a). On one hand, observed F_C has great variability at hourly scale throughout the year indicated by the large ~~deviation~~ interquartile range (Fig. 6). On the other, under the current parameterization, two of the anthropogenic F_C components are static: modelled traffic emission diurnal cycle is only dependent on whether it is weekend or weekday, and modelled human metabolism diurnal cycle is invariable throughout the year (Fig. 7), making it difficult to capture the extreme values. Other urban F_C bottom-up modelling studies also reported similar challenges in modelling F_C hourly variability in ~~Basel and in Helsinki (Stagakis et al., 2022; Järvi et al., 2019)~~ Helsinki and in Basel (Järvi et al., 2019; Stagakis et al., 2022).

SUEWS gives a reasonable estimate of annual accumulated F_C (~~8.4~~ 8.6 kg C m^{-2} yr^{-1}), which is ~~12~~15% higher than the observed gap-filled value (7.5 kg C m^{-2} yr^{-1}). F_C is ~~overall slightly underestimated in winter months (with MBE around -0.7~~ overestimated in all seasons, with the lowest MBE (0.2 μmol m^{-2} s^{-1}) ~~while overestimated in the other seasons, with the largest MBE (4.6–5.5~~ in winter and the highest MBE (5.7 μmol m^{-2} s^{-1}) in summer (Fig. 8 c). ~~SUEWS overestimates summer~~

There are multiple reasons to explain the difficulty in accurately capturing the diurnal cycle of the observed F_C ~~, which might be explained by the underestimation of~~ for each season. First, the influence of the underlying seasonal variation in the diurnal wind pattern is not considered. The observed F_C varies noticeably with wind direction, and at the same time, the diurnal cycle of wind direction frequency varies with season. This makes the F_C diurnal cycle from the NW quadrant more "seen" in winter and spring, while the diurnal cycle from SE more "seen" in summer and autumn (Fig. S2). SUEWS cannot consider this F_C's wind-direction dependency as it simulates the overall flux from the simulation domain. Second, atmospheric stability influences the real-time footprint fetch of F_C (Crawford and Christen, 2015), but this is not considered in our study. Third, there might be biases in simulating the seasonal cycles of F_C components. SUEWS might underestimate the vegetation photosynthetic rate or overestimate the CO$_2$ release from respiration due to the lack of site-specific ~~parameters.~~ biogenic parameters. Nonetheless, the model performance over the F_C diurnal cycle is reasonably good as compared to a previous study (Järvi et al., 2019).
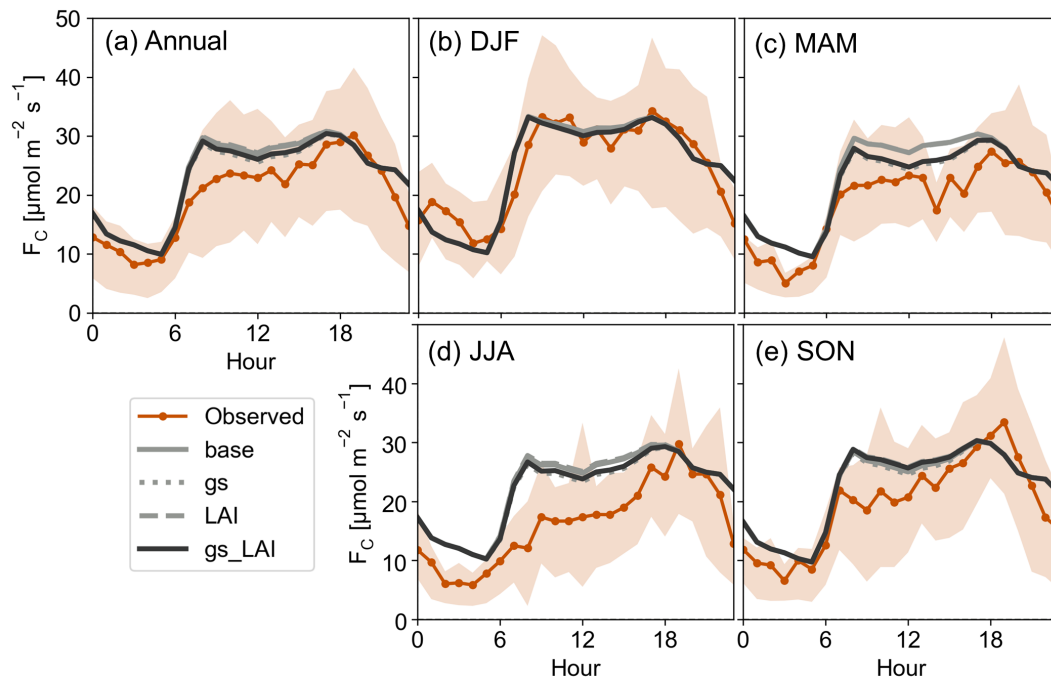
Figure 6. Annual and seasonal average diurnal cycles of observed and modelled CO$_2$ flux (F_C) for the four model ~~runs~~ cases (case **base**, **gs**, **LAI**, and **gs_LAI**) in the year 2016. The shaded area denotes the interquartile range.
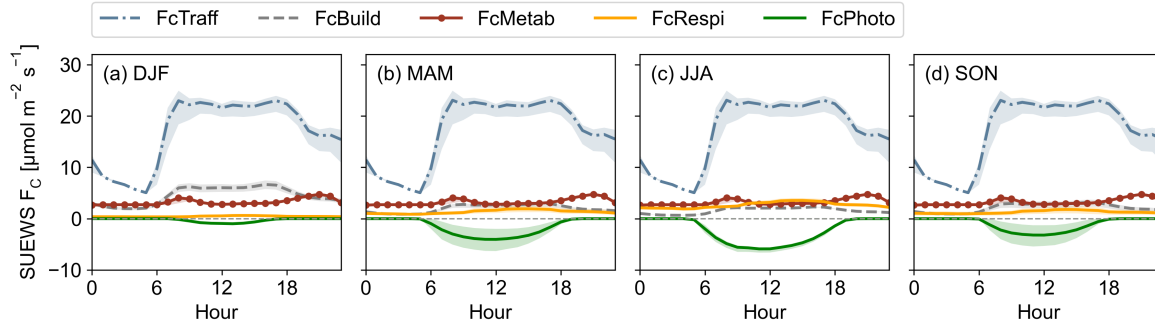
Figure 7. Seasonal average diurnal cycles of modelled CO_2 flux (F_C) components by case **gs_LAI** in 2016. FcTraff denotes ~~the~~ CO_2 emissions from on-road traffic, FcBuilding building, FcMetab human metabolism, FcRespi vegetation and soil respiration, and FcPhoto ~~the~~ CO_2 uptake by vegetation photosynthesis. Positive values indicate ~~sources~~ the emissions of CO_2 and negative values ~~sinks~~ indicate the uptake of CO_2 with respect to the atmosphere. The shaded area denotes the interquartile range.
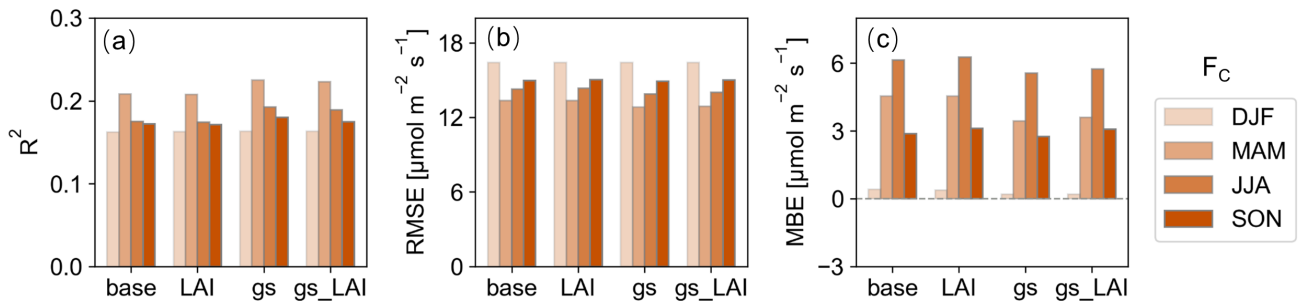
Figure 8. Model performance statistics (a) R^2, (b) RMSE and (c) MBE of CO_2 flux (F_C) for the four cases (**base**, **gs**, **LAI**, and **gs_LAI**) in the year 2016.

5.3.2 ~~Model uncertainties~~

Uncertainties in traffic emission originate from the traffic rates and EFs. SUEWS adopts static traffic EFs, and neglects the relationship between traffic emission and T_{air} as reported by Alvarez and Weilenmann (2012) and Fontaras et al. (2017). In order to examine the impact of seasonal variation of T_{air} in traffic emission, correction is conducted using the regression function following Zhang et al. (2021), but only a marginal difference is seen at monthly scale: a difference of 3% in winter, -2% in spring, ~0% in summer and -1% in autumn. Therefore, we believe that the static traffic EFs adopted by SUEWS can provide reasonable traffic emission without considering the seasonal dynamics of T_{air}.

Järvi et al. (2019) reported that using a different coefficient of CO_2 release per capita (C_M) lead to a 6% decrease in human metabolic CO_2 emission estimate. If C_M is set to a daily mean value of 242 μmol m^{-2} s^{-1} (Prairie and Duarte, 2007) instead

of the current values (Table 1), the human metabolic emission will increase and the annual F_C will be 4% higher than the original estimate.

Building ~~emission~~ emissions are calculated based on the Q_F estimates and heating fraction. Modelled average Q_F in December is 52.7 W m^{-2}, which is higher than another model estimate (21.6 W m^{-2}) in the modelled area (Wang et al., 2020). Observations of Q_F are rarely available, and thus these Q_F estimates have not yet been validated. The representativeness of the heating fraction estimated from yearbook statistics is yet to be examined because the location and heating capacity of heating boilers within the modelled area is unknown. However, the building emission estimate (~~0.6~~0.97 kg C m^{-2} yr^{-1}) falls in the range of estimates (~0–3.0 kg C m^{-2} yr^{-1}) by other cities ~~(Björkegren and Grimmond, 2018; Järvi et al., 2019; Moriwaki and Kanda, 2004; Christen~~ (Björkegren and Grimmond, 2018; Christen et al., 2011; Järvi et al., 2019; Moriwaki and Kanda, 2004).

The modelled CO_2 release by respiration is larger than CO_2 assimilated through photosynthesis in our study. At the annual scale, urban vegetative surfaces can ~~serve as~~ have a net CO_2 ~~sink~~ uptake (Awal et al., 2010; Konopka et al., 2021), but may also ~~vary from a net CO_2 sink to a source~~ have a net emission (Peters and McFadden, 2012). Admittedly, bias might exist in biogenic CO_2 flux estimates since the parameters used in this study are derived from the observations over street trees in Helsinki and over a lawn at Ossinlampi, Finland, where the climate and vegetative species are different from Beijing. With these parameters, the model might underestimate the CO_2 sequestered by the local vegetation, ~~and overestimate net F_C in the growing season as shown in Sect. 5.3.1.~~ or overestimate the CO_2 release by respiration.

5.3.2 The impact of the modelling domain size

The surroundings of ~~the~~ IAP tower are heterogeneous in terms of land surface fraction and mean daily traffic rate (Fig. 9 a). The fraction of vegetated surfaces is higher closer to the tower than further away due to the green spaces adjoining ~~the~~ IAP tower (Fig. 1 b). Additionally, there is a traffic hot spot on the ~~North~~ 3rd Ring North Road located 850 m to the south of IAP tower (Fig. 1 d), where the traffic rate is 2 to 7 times the value for the other roads inside the circle of a 1000 m radius (figure not shown). A large increase of 26% in daily traffic rate is seen when the radius of modelling domain is 1000 m or 1500 m when compared to domains with lower radii (Fig. 9 a). Thus, the modelled annual accumulated F_C largely depends on the modelling domain size chosen, giving estimates of ~~7.2,~~ 7.4, ~~8.4 and 8.5~~ 7.6, 8.6 and 8.7 kg C m^{-2} yr^{-1} for the radii of 500 m, 750 m, 1000 m, and 1500 m, respectively. Observational annual F_C (7.5 kg C m^{-2} yr^{-1}) falls within this range, which indicates the good model performance of SUEWS (Fig. 9 b).

~~Land surface fractions are critical parameters in~~ The turbulent flux modelling ~~, but the use of site-specific fractions covering a certain area might not yield the best model performance (Demuzere et al., 2017; Loridan and Grimmond, 2012). Approximating the source area by choosing the radius of~~ is usually evaluated over a fixed extent such as a circle with a certain radius to approximate the flux source area (Demuzere et al., 2017; Järvi et al., 2019). However, when a circle with the radius $\geq$ 1000 m is selected to approximate the $\geq$80% footprint fetch ~~(i.e. $\geq$1000 m in this study)~~ in our study, SUEWS does not give the closest estimate of annual F_C ~~, showing agreement with previous studies. The model performance on heat and F_C fluxes is reasonably good for each radius (figure not shown), but the selection of radius causes a difference up to 17.5% on annual F_C estimate (Fig. 9b). .~~ This can be explained by the mismatch between the modelling domain and the real flux source

520 area—the single fixed-extent modelled area cannot perfectly represent the land surface characteristics (e.g., the nonuniform land cover and human activities), biasing turbulent flux modelling (Chu et al., 2021; Laine et al., 2009). First, the accumulated footprint area of the observed fluxes is irregular in shape and vary with time (Liu et al., 2012)~~, while many studies (Demuzere et al., 2017; Järvi et al., 2019) including this study select a circular area to be modelled and evaluated. Changing the size of modelling domain is challenging when soil processes are taken into account in SUEWS.~~. Second, the relative con-

525 tribution to flux from the land surface decreases as the distance to the measurement instrument increases (Christen et al., 2011; Rebmann et al., 2005). ~~When~~ Thus, when the modelling domain is a 1000 m radius circle, the model might underestimate the relative contribution from the adjacent vegetated surface, and overestimate the contribution of the traffic hot spot at the edge of 80% footprint fetch. ~~We conclude that the land surface model single-point evaluation needs to be performed with the awareness of the mismatch between flux source area and modelling domain, especially over heterogeneous surfaces such as~~

530 ~~urban surfaces.~~
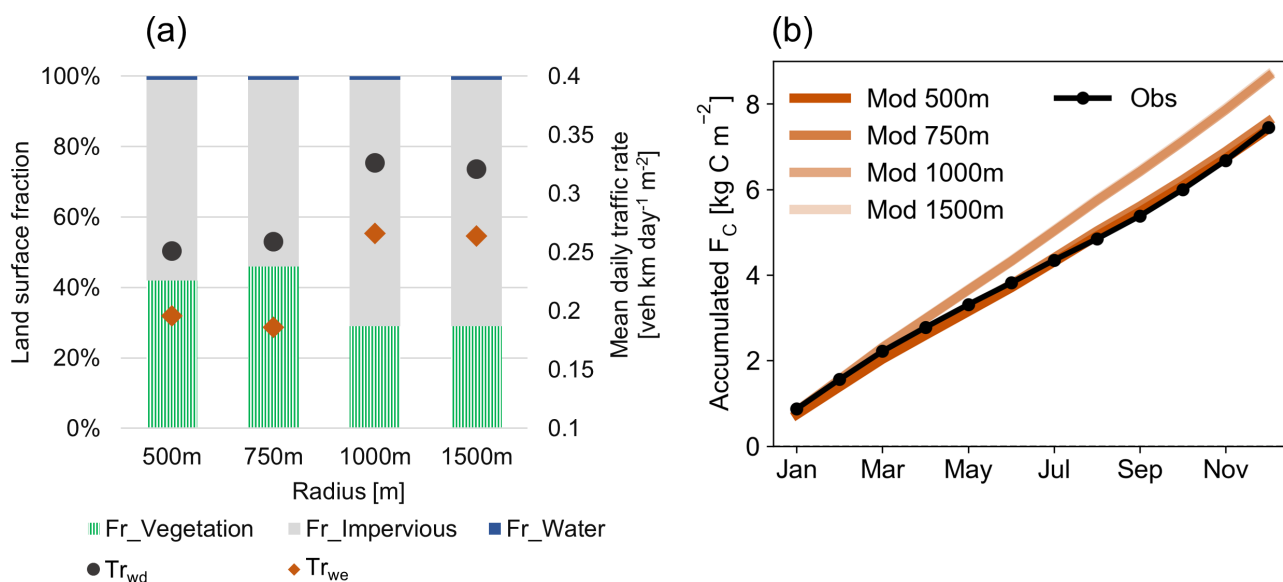
Figure 9. (a) Land use fraction and mean daily traffic rate (~~VKT, same as Tr in Table 1~~$Tr_{wd/we}$), and (b) accumulated CO$_2$ flux (F_C) for modelling domain with the radius ranging from 500 m to 1500 m. "~~WD~~Wd" denotes weekday, "~~WE~~we" weekend; "Mod" denotes modelled F_C, and "Obs" observed F_C. Note that in (b) the lines for Mod 500m and Mod 750 m nearly overlap, and the lines for Mod 1000m and Mod 1500m nearly overlap.

Regardless of the modelling domain size, traffic is the dominant CO$_2$ source~~contributing 63–73~~, contributing 59–70% to the total CO$_2$ emissions, followed by human metabolism (14–18%), ~~respiration released by vegetation and soil (6–11~~building energy use (11–14%), and ~~heating (6–9~~CO$_2$ release by vegetation and soil respiration (6–10%). Vegetation photosynthesis offsets only ~~4–8~~5–10% of the total annual CO$_2$ emissions (Fig. 10). Several bottom-up modelling studies show that

535 the on-road traffic is the greatest source in a densely built neighbourhood, contributing to 70% in central London, 61% in

Helsinki, 53%–78% in Tokyo, 70% in Vancouver, while human metabolism also plays an important role, contributing 5–39% to the annual total F_C ~~(Björkegren and Grimmond, 2018; Järvi et al., 2019; Moriwaki and Kanda, 2004; Christen et al., 2011)~~ (Björkegren and Grimmond, 2018; Christen et al., 2011; Järvi et al., 2019; Moriwaki and Kanda, 2004). Our results are in general agreement with these studies. The contribution of ~~building emission~~ the local building emissions within the study area is

540 more variable among cities: a contribution of 70% is reported in Basel (Stagakis et al., 2022), while ~0% in Helsinki (Järvi et al., 2019), and our estimate falls in this range. The direct CO_2 sequestration by urban plants is minor compared with the total CO_2 emissions in this densely built ~~neighborhood~~neighbourhood, which is in general agreement with Pataki et al. (2011) and Christen et al. (2011). For more accurate biogenic component estimates in Beijing, photosynthetic and respiration observations over local species are needed in the future.
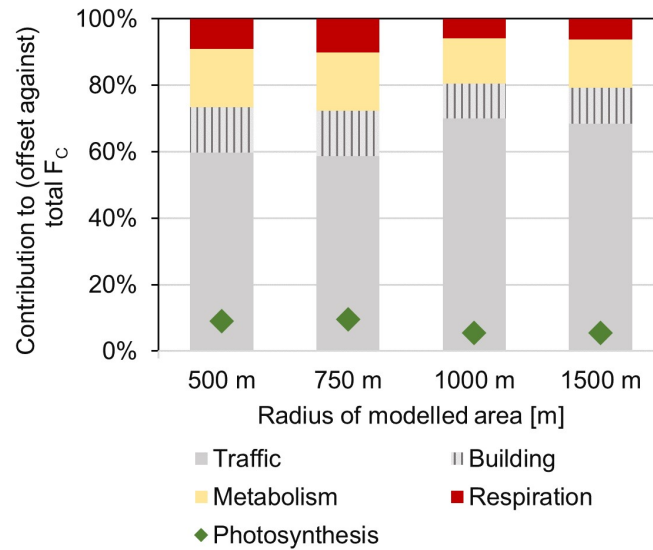
Figure 10. The contribution to total CO_2 emissions by each component at the annual scale for the modelled area with a radius ranging from 500 m to 1500 m. Note that for photosynthesis the percentages denote the offset against total CO_2 emissions.

545 **6 Conclusions**

A correct description of vegetation is vital in order to simulate the energy and CO_2 fluxes over urban surfaces using the urban land surface model SUEWS. In this study, the impact of selecting appropriate vegetation parameters, including LAI parameters and g_{max}, on simulating the surface fluxes is examined in Beijing, China. Besides, the newly-developed CO_2 emissions module in SUEWS is evaluated against EC measurements.

550 ~~Radiation flux modelling performs well without fine-tuning and it is hardly influenced by g_{max} and LAI. The modelling~~ The model performance of heat fluxes ~~including~~ (Q_E and Q_H~~, however, shows great sensitivity to~~) is more sensitive to the adjustment of g_{max} ~~and the behaviour of LAI . LAI model~~ than to the change of LAI seasonal dynamics in our study

area. The LAI model has been improved by using ~~"default" parameters from previous studies has difficulty in capturing the phenology dynamics (e.g., the rate of leaf-growth, leaf-off) in Beijing, likely due to the dry-wet season pattern. By using~~ CMA-ES to optimize the LAI parameters with a remotely sensed LAI ~~, the LAI modelling is noticeably improved (R^2=0.94, RMSE=0.4 m^2 m^{-2})~~product, providing more realistic vegetation phenological dynamics, especially for the senescence season. Observational leaf-level g_{max} of vegetative species in Beijing are also collected and parameterized. By incorporating local LAI and g_{max}, SUEWS ~~simulated~~ simulates the heat fluxes ~~remarkably~~ noticeably better, increasing R^2 by ~~0.02 (0.36~~0.03 (0.30) and decreasing RMSE by ~~27.4 (27.9~~27.0 (23.7) W m^{-2} for Q_E (Q_H), and showing more realistic seasonal dynamics when compared to EC observations.

~~In comparison of heat flux modelling,~~ F_C modelling ~~shows lower sensitivity to the choice~~ appears to be less sensitive to the choices of LAI-related parameters and g_{max}. Only one of the F_C components, F_{pho}, responds noticeably to them. SUEWS can catch the general diurnal and seasonal behaviour of F_C but tends to overestimate F_C, especially over summer months. We also tested the influence of chosen modelling domain size on simulated F_C. By selecting the modelled radii of circular area ranging from 500 m to 1500 m (i.e., accumulated footprint area from 60% to 80–90%), the modelled annual F_C ranges from ~~7.2 to 8.5~~7.4 to 8.7 kg C m^{-2} yr^{-1}, which is comparable with the EC observations (7.5 kg C m^{-2} yr^{-1}). This shows the model performs well also on the annual scale. ~~The variation in annual cumulative F_C with radii can be explained by spatial heterogeneity over the urban landscape, and the mismatch between the modelling domain and flux source area.~~ Regardless of the modelling domain size, traffic is the dominant CO_2 source, contributing ~~63–73~~59–70% to the total CO_2 emissions, followed by metabolism (14–18%), ~~respiration released by vegetation and soil (6–11~~building (11–14%), and ~~heating (6–9~~CO_2 release by vegetation and soil respiration (6–10%). Vegetation photosynthesis offsets only ~~4–8~~5–10% of the CO_2 emissions.

We highlight the importance in choosing more site-specific LAI parameters or g_{max} when ~~using SUEWS in modelling heat fluxes , before~~ SUEWS is used for heat fluxes modelling before the more advanced application ~~regarding~~ such as urban climate and hydrological modelling. Observations are needed to support more accurate parameterizations of biogenic CO_2 fluxes. We believe that the bottom-up approach to model F_C by SUEWS can be a promising tool in ~~quantifying urban CO_2 emissions at the local scale, and therefore apply to capture the~~ capturing the CO_2 emission hot ~~spot, quantifying~~spots, quantifying the relative contribution of the local CO_2 sources, and ~~assist~~ assisting to mitigate urban CO_2 emissions.

Appendix A: Workflow of LAI parameters optimization

In SUEWS, LAI influences the surface conductance, and subsequently Q_E and F_{pho} (Sect. 2). A workflow for parameter derivation for the LAI sub-model based on remotely-sensed data is designed for natural ecosystems (Omidvar et al., 2022). However, vegetation in urban areas behaves differently from natural ecosystems (Zhang et al., 2022), and needs to be considered separately. Therefore, we propose a workflow to obtain the parameters for urban area based on remotely-sensed LAI and Covariance matric adaptation evolution strategy (CMA-ES). This workflow can also be applied to natural ecosystems. The related data and codes are openly available (Zheng et al., 2022).

585 Covariance matric adaptation evolution strategy (CMA-ES) is one of the strategies for numerical optimization of non-convex problems. It is based on the principle of biological evolution. The evolution strategy takes a certain number of individuals (candidate solutions) in a stochastic way, selects individuals based on the fitness, and repeats this process for generations so that a better or an optimal solution is obtained. Adaptation of the covariance matrix amounts to learning a second order model of the underlying objective function. Compared with classic optimization methods, CMA-ES requires neither derivatives nor an

590 objective function; it only requires the ranking of candidate solutions. Besides, CMA-ES outranks many of other optimization algorithms, performing especially strong on "difficult functions" or larger dimensional search spaces (Hansen et al., 2010).

Taking ~~Beijing~~ our study area as an example, the LAI parameters are optimized as the following:

1. ~~City-level~~ LAI derivation. ~~The NASA Moderate Resolution Imaging Spectroradiometer (MODIS) product MOD15A2H with 8-day and 500-m resolution is first derived. The spatial average of LAI within the 6th ring area of Beijing is extracted~~

595 ~~from the year 2008 to 2016,~~ A six-year time series (2011–2016) of LAI of the vegetation in an adjacent park near IAP tower is calculated from the atmospherically corrected surface reflectance provided by USGS Landsat 7 Enhanced Thematic Mapper + (ETM+) (30 m spatial resolution) via the Google Earth Engine Data Catalog (Masek et al., 2006). The time series is treated as the ~~city-level of LAI~~ "original LAI".

2. Spikes removal. There are outliers in the LAI time series caused by instrument problems, uncertainties of retrieval

600 algorithm, and cloud contamination. Values larger than 10 $m^2\ m^{-2}$ and negative values are first removed. The LAI values during December and January are set to a fixed value, i.e., the average of these months (0.2 $m^2\ m^{-2}$), in order to reduce the noise in winter and improve the optimization performance.

3. Scaling ~~city-level~~ the original LAI to the ~~tree-level. We note that the city-level~~ canopy level. The original LAI might be noticeably lower than the ~~LAI at tree level due to the presence of non-vegetated surfaces in urban area~~ measured

605 LAI at the canopy level over a homogeneous vegetated surface. Nonetheless, the ~~city-level~~ original LAI provides the signals of vegetation phenology (e.g., leaf-out, peak growing season, leaf-fall). In order to give a more realistic estimate of LAI at the ~~tree-level, the LAI city-level~~ canopy level, the original LAI needs to be scaled. Therefore, LAI_{max} and LAI_{min} need to be given manually, preferably based on observational studies over local species. ~~An observational study in Beijing shows that the maximum of LAI falls between 5 and 6~~ Here, the original LAI is scaled to allow the optimized

610 LAI to reach 5–6 $m^2\ m^{-2}$ (Wang et al., 2021). Here, LAI_{max} = 6 and LAI_{min} = 0.1 $m^2\ m^{-2}$.

4. ~~Spikes removal. Spikes occur occasionally due to instrument problems, uncertainties of retrieval algorithm and cloud contamination. Therefore, data points are identified as spikes if:~~

$$\left| LAI - LAI_5 \right| > \frac{\sqrt{LAI + LAI_5}}{\beta},$$

~~where LAI_5 is the moving median of 5 consecutive data points, and β is constraint factor (here $\beta = 2$). The spikes are~~

615 ~~removed, marked as~~ in the peak growing season as reported by an observational study in Beijing (Wang et al., 2021). The

canopy-level LAI is marked as the "~~sample discarded~~input LAI" ~~; the other sample are kept, marked as~~ for the process of optimization and marked as the "~~sample retained" and treated as~~ "observed LAI" ~~. In the case shown here, 7 data points are discarded, accounting for 1.7% of the total sample.~~

for the process of evaluation.

5. Interpolation. The observed LAI are linearly interpolated between values to obtain a daily time series, marked as the "interpolated LAI".

6. Parameters derivation using CMA-ES. The time series of interpolated LAI and T_{air} are subjected to CMA-ES to optimize the parameters. Using the LAI model and the parameters derived, LAI is calculated and marked as the "predicted LAI".

~~LAI model incorporated with the optimized parameters successfully reproduces the seasonal dynamics of observed LAI, capturing the timing of growth, peak growing season, and senescence.~~ The input LAI fluctuates greatly in summer, but the CMA-ES method provides a good estimate of the LAI seasonal dynamics, indicating that the CMA-ES is a useful tool that can handle input data contaminated by noise (Fig. A1 a). The model performance is ~~remarkably good , with high~~ overall good (with R^2 ~~(0.94) and low RMSE (0.4~~ = 0.74 and RMSE = 1.2 m^2 m^{-2}) (Fig. A1 b).
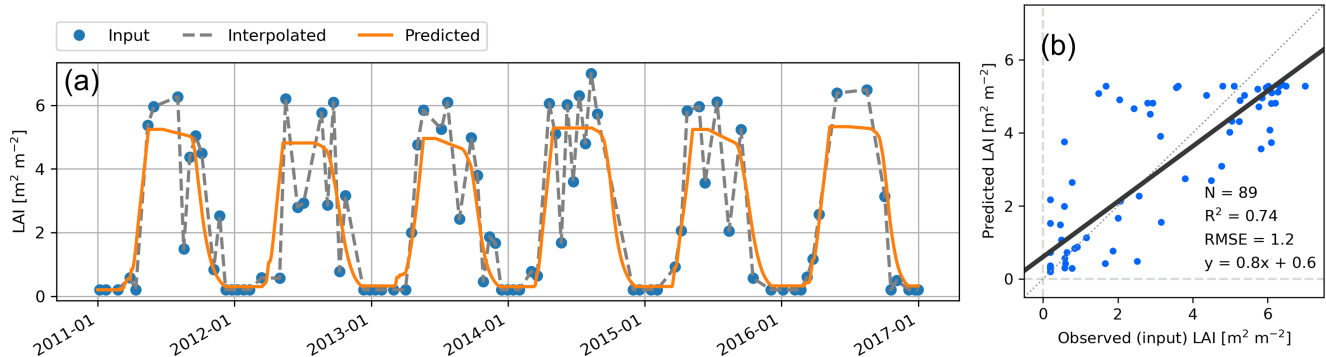
Figure A1. (a) Time series of the ~~the~~ input, the interpolated, and the predicted leaf area index (LAI)~~sample retained~~, ~~LAI sample discarded, interpolated LAI~~ and ~~predicted LAI, and~~ (b) comparison of the predicted against the observed LAI.

Appendix B: Evaluation of WFDE5 reanalysis against observed meteorological variables

To force SUEWS, local scale meteorological data within the inertial sublayer is required. However, they can be unavailable for the area and period desired. Reanalyses provide spatially and temporally complete datasets, which might make the modelling run easier for users. Kokkonen et al. (2018) and Kokkonen et al. (2019) evaluated one of the reanalyses, WATCH Forcing Data ERA-Interim (WFDEI), suggesting that WFDEI can serve as the forcing of SUEWS, but should be corrected beforehand when the bias is large.

635 WFDE5 is a bias-corrected dataset of near-surface meteorological variables derived from the fifth generation of the European Centre for Medium-Range Weather Forecasts (ECMWF) atmospheric reanalysis (ERA5) (Cucchi et al., 2021). It is generated using the same methodology as WFDEI, and provides a single layer at 0.5° spatial resolution and hourly temporal resolution. The evaluation of WFDE5 and the use of it as forcing data to SUEWS have been neglected so far. Here, we compare WFDE5 against observed meteorological variables including air temperature (T_{air}), relative humidity (RH), wind velocity (U) at 47 m,

640 and incoming shortwave radiation (K_{down}) at 140 m on ~~the~~ IAP tower (Liu et al., 2012). The evaluation of K_{down} is conducted from May 2010 to June 2011, and the rest from January 2010 to December 2011. All the observed variables are resampled from 30-minute to 1-hour resolution.

Table B1. The height of WFDE5 and observed meteorological variables.

	WFDE5	Observations
T_{air}	2 m	47 m
RH	near surface	32 m
U	10 m	47 m
K_{down}	near surface	140 m

 With the difference in height for each meteorological variable (Table B1), however, WFDE5 is close to the observed as a whole (Fig. B1). Compared with the observed, WFDE5 T_{air} is lower, RH higher, U lower, and K_{down} higher. WFDE5 may

645 underestimate T_{air}, and overestimate RH, for neglecting the urban anthropogenic heat release; WFDE5 might overestimate K_{down} due to insufficient consideration of aerosol's effect in decreasing solar radiation received by the urban surface. The lower U of WFDE5 can be explained by the lower height compared with the observations (Table B1). If the WFDE5 U is adopted as forcing of SUEWS, aerodynamic resistance might be overestimated, and therefore Q_E underestimated.

 Admittedly, some meteorological variables of WFDE5 correlate poorly with the observations in a particular season (e.g.,

650 R^2=0.13 for U in JJA). However, the overall high R^2, and low RMSE and MBE in magnitude suggest that WFDE5 provides reasonably good estimates of each meteorological variable (Table B2). Therefore, WFDE5 is adopted as the forcing data of SUEWS in this study.
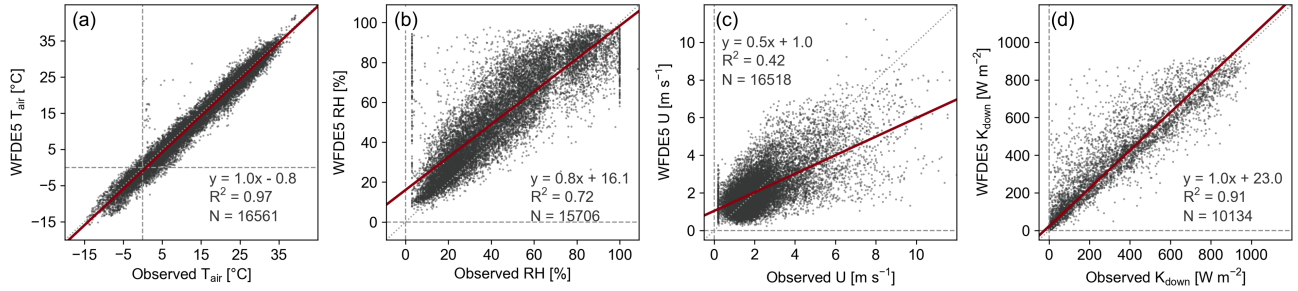
Figure B1. Comparison of WFDE5 and observed meteorological variables including (a) air temperature (T_{air}), (b) relative humidity (RH), (c) wind velocity (U) and (d) incoming solar radiation (K_{down}) at an hourly resolution.

Table B2. Statistics for WFDE5 compared against the observed meteorological variables.

	Season	average		R^2	RMSE	MBE	N
		WFDE5	Observed				
T_{air} (°C)	DJF	-2.1	-1.2	0.83	2.3	-1.0	4217
	MAM	12.7	13.5	0.92	2.5	-1.0	4100
	JJA	26.2	26.8	0.77	2.1	-0.5	3966
	SON	13.8	14.2	0.94	1.9	-0.4	4278
RH (%)	DJF	41.8	32.4	0.77	13.4	9.3	4216
	MAM	41.6	34.1	0.74	13.8	7.9	3986
	JJA	66.6	59.9	0.71	12.6	5.1	3546
	SON	60.2	49.3	0.50	20.6	10.9	3958
U (m s^{-1})	DJF	2.1	2.7	0.52	1.3	-0.5	4217
	MAM	2.7	2.8	0.45	1.4	-0.1	4100
	JJA	1.9	1.9	0.13	1.2	0.1	3949
	SON	2.0	1.9	0.45	1.0	0.0	4252
K_{down} (W m^{-2})	DJF	117.0	99.2	0.94	50.6	19.5	2160
	MAM	222.5	218.1	0.93	82.7	19.7	2941
	JJA	216.4	189.3	0.86	110.5	38.2	2883
	SON	140.9	124.7	0.93	58.9	16.5	2150

Appendix C: Evaluation of radiation fluxes

The radiation parameterization scheme Net All-wave Radiation Parameterization (NARP) does not involve g_{max} or LAI. As expected, the four experiments (Sect. 4.5.1) give identical radiation flux components in the output. Therefore, only the case **gs_LAI** is further analyzed here.

The model performance of SUEWS in simulating radiation fluxes is good (Fig. C1, Table C1) and it can reproduce the diurnal cycle of each radiation flux well (Fig. C2). K_{up} is overestimated in all seasons with MBE ranging from 0 to 10 W m^{-2}. At least partly, this overestimation can be explained by the positive bias (MBE > 15 W m^{-2} in all seasons) of WFDE5 K_{down} when compared to the observed K_{down} (Appendix B). The overestimation in K_{up} can also be caused by surface albedo. Observational studies have shown that the urban surface albedo near IAP tower varies between 0.1 and 0.15 with season (Jiang et al., 2007; Miao et al., 2012). The annual bulk albedo for the modelling domain given to SUEWS is 0.14, which is relatively high but still consistent with the observations. A larger positive bias in K_{up} is observed in summer than in winter. Surface albedo is influenced by many factors such as surface wetness and street canyon trapping effect (Ao et al., 2016; Dou et al., 2019), which have not yet been considered by SUEWS. By simply (1) adjusting the albedos for surface types following Ward et al. (2016), and (2) allowing albedo for vegetation to vary from a lower value in summer to a higher value in winter (Table S5), the RMSE for K_{up} decreases for all seasons, especially in summer (from 18.0 to 13.6 W m^{-2}), but this has only a minor impact on Q_N modelling (Table S6).
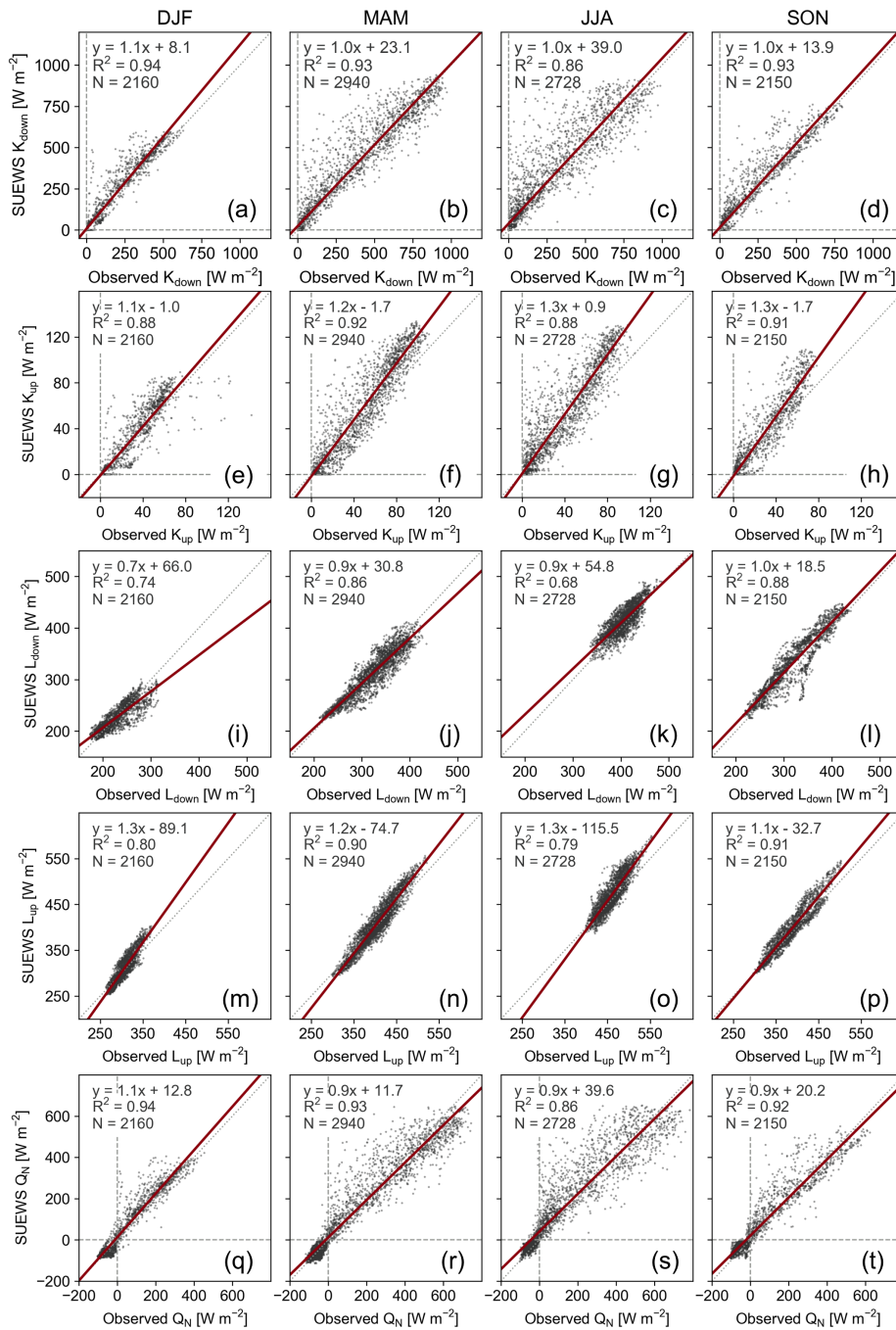
Figure C1. Input or modelled vs. observed hourly radiation fluxes, including (a–d) incoming solar radiation (K_{down}), (e–h) outgoing shortwave radiation (K_{up}), (i–l) incoming longwave radiation (L_{up}), (m–p) outgoing longwave radiation (L_{up}), and (q–t) net radiation (Q_N) from May 2010 to June 2011. Note that only K_{down} is input and the rest are model output.
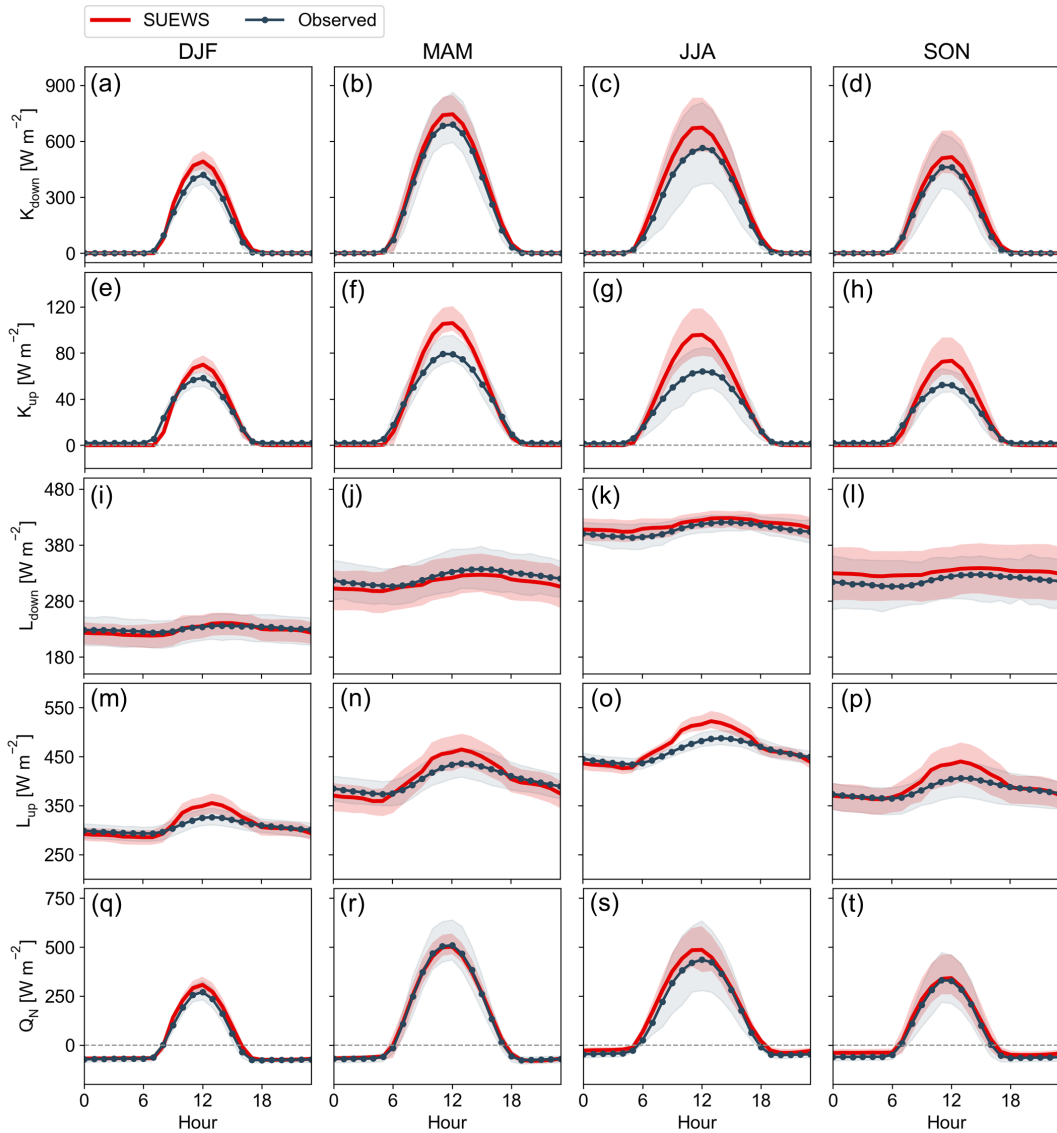
Figure C2. Average diurnal cycle of input or modelled and observed hourly radiation fluxes by season, including (a–d) incoming solar radiation (K_{down}), (e–h) outgoing shortwave radiation (K_{up}), (i–l) incoming longwave radiation (L_{up}), (m–p) outgoing longwave radiation (L_{up}), and (q–t) net radiation (Q_N) from May 2010 to June 2011. Shading area denotes the standard deviation. Note that only K_{down} is input and the rest are model output.

The average seasonal and diurnal cycles of L_{down} are well captured by the model (Fig. C2 i–l), although R^2 (0.68–0.88) is lower than with other radiation fluxes. The difference might result from the discrepancy between the observed and modelled cloud fraction as clear skies and overcast conditions are especially difficult to capture by the radiation model NARP, as reported also by Ao et al. (2016) and Ward et al. (2016). The diurnal amplitude of L_{up} is slightly overestimated by SUEWS (Fig. C2

670

m–p). The model tends to overestimate L_{up} particularly at high values of L_{up} (Fig. C1 m–p). The values of emissivity of building materials used in SUEWS might be slightly higher than in reality. L_{up} is also dependent on K_{down} in NARP.

675 Therefore, the overestimation of L_{up} can be partly explained by the overestimated K_{down} provided by WFDE5, especially around noon and in summer.

We conclude that SUEWS is applicable to provide a realistic estimate of radiation fluxes in Beijing, in general accordance with previous studies (Järvi et al., 2014; Karsisto et al., 2016; Ward et al., 2016), despite the absence of site-specific parameters.

Table C1. SUEWS model performance statistics for radiation fluxes. The abbreviations are the same as Fig. C1. Note that K_{down} is an input and others are output of SUEWS.

	Season	R^2	RMSE	MBE	N
K_{down}	DJF	0.94	52.3	19.5	2160
	MAM	0.93	82.6	19.8	2940
	JJA	0.86	110.4	39.3	2728
	SON	0.93	59.6	16.6	2150
K_{up}	DJF	0.88	9.2	0.2	2160
	MAM	0.92	14.8	5.0	2940
	JJA	0.88	18.0	8.1	2728
	SON	0.91	11.6	3.3	2150
L_{down}	DJF	0.74	16.0	-2.4	2160
	MAM	0.86	20.5	-10.0	2940
	JJA	0.68	18.1	8.8	2728
	SON	0.88	23.7	12.9	2150
L_{up}	DJF	0.80	15.3	3.8	2160
	MAM	0.90	18.6	3.2	2940
	JJA	0.79	22.1	10.5	2728
	SON	0.91	18.6	9.2	2150
Q_N	DJF	0.94	38.0	13.2	2160
	MAM	0.93	64.6	1.5	2940
	JJA	0.86	87.0	29.5	2728
	SON	0.92	50.8	17.0	2150

Appendix D: Fitting maximum photosynthetic rate for vegetation type of grass/lawn

In order to find the maximum photosynthetic rate for the vegetation type of grass to be used in SUEWS simulation, the environmental response functions $g(T_{air})$, $g(\Delta q)$, $g(\Delta\theta)$, and $g(K_{down})$ in Eq. 14 were fitted to observations from an eddy covariance (EC) station (60°11'16.02"N, 24°49'56.85"E) situated in an urban lawn in Espoo, Finland. A 1.2 m high EC tower was located at the center of the urban lawn covering an area of 0.7 ha. The EC setup consisted of a three-dimensional sonic anemometer (Metek GmbH, Germany) for measuring the three wind components and sonic temperature, and a closed-path infrared gas analyser (LI-7200; LI-COR, Lincoln, NE, USA) for measuring the CO_2 and H_2O mixing ratios. The gas analyser inlet was positioned 13 cm below the anemometer and air was drawn into the gas analyser using a 60 cm length of steel tube, having an inner diameter of 4.57 mm and a mean flow rate of $12\,l\,min^{-1}$. The tube was heated to avoid water vapor condensation on tube walls. The raw EC data were sampled at 10 Hz and stored for post-processing. The steps before 30-min flux calculations consisted of de-spiking, linear de-trending, and planar fitting of the raw data.

The biogenic CO_2 flux $F_{c,bio}$ from EC measurements was partitioned into F_{res} and F_{pho} using the night-time temperature dependency of F_{res}. The nighttime $F_{c,bio}$ was considered as nighttime F_{res}, and it was related to the observed T_{air} by fitting the exponential model:

$$F_{res} = a_{grass} \cdot exp\left(T_{air} b_{grass}\right), \tag{D1}$$

where a_{grass} and b_{grass} are parameters controlling the temperature dependency. The nighttime temperature dependency of F_{res} was then extrapolated to daytime, and F_{pho} was then calculated by

$$F_{pho} = F_{C,bio} - F_{res}. \tag{D2}$$

Then F_{pho} was used as a dependent variable, whereas on-site measurements of net radiation (CNR4; Kipp&Zonen, Delft, Netherlands), air temperature, and relative humidity (HMP110 A15; Vaisala Oyj, Vantaa, Finland) and soil moisture (ML3 Thetaprobe; Delta-T, Cambridge, UK) were used to estimate the independent variables in $g(T_{air})$, $g(\Delta q)$, $g(\Delta\theta)$ and $g(K_{down})$. Atmospheric pressure from Finnish Meteorological Institute Kumpula station was used to calculate Δq. Additional reference values of soil properties (field capacity and wilting point), which were estimated to be same as in an urban lawn in Kumpula (Järvi et al., 2019), were used to calculate $\Delta\theta_{WP}$. Parameters $F_{pho,max}$ and $G_2 - G_6$ were fitted using a non-linear least-square approach.

Data from mid-July to the end of August 2021 were used and in the fitting only data points with $K_{down} > 10$ W m^{-2} and $\Delta q > 1$ g kg^{-1} were selected (Havu et al., 2022a). After applying a bootstrapping method to randomly select seven eighths of the data for 100 times, the final parameters fitted for grass were obtained as medians with the uncertainties as follows: $F_{pho,max} = 5.497 \pm 0.110\,\mu$mol m^{-2}s^{-1}, $G_2 = 195.019 \pm 5.601$ W m^{-2}, $G_3 = 0.741 \pm 0.008$, $G_4 = 0.413 \pm 0.015$, $G_5 = 30.000 \pm 0.000$ °C, $G_6 = 0.500 \pm 0.000$ mm^{-1}. The value of $F_{pho,max}$ is used for grass/lawn in the Beijing simulation.

Appendix E: Maximum conductance of urban green space in Beijing

Table E1. Maximum conductance (g_{max}) for each vegetated surface.

	Deciduous tree			
	Sophora japonica Linn.	*Populus tomentosa* Carr.	*Faxinus chinensis* Roxb.	*Ginkgo biloba* Linn.
Ratio[a]	26.26%	12.39%	9.44%	8.12%
g_{max} (mm s^{-1})	9.0	5.2	6.1	4.1
Reference	Xu et al. (2020)	Wang et al. (2018)	Xu et al. (2020)	Song et al. (2015)
	Evergreen tree	Grass/lawn		
	Pinus tabuliformis	*Festuca arundinacea* Schreb.	*Poa pratensis* L.	*Zoysia japonica* Steud.
g_{max} (mm s^{-1})	1.4[b]	5.4	4.0	1.6
Reference	Chen et al. (2021)	Wang et al. (2006)	Wang et al. (2006)	Wang et al. (2006)

[a] obtained from a field survey over Beijing (Ma et al., 2019)

[b] obtained by dividing maximum canopy conductance by G_1 (=3.5)

The weighted average of g_{max} is 7.0 mm s^{-1} for the deciduous tree weighted by the population ratio of each species (Table E1). The average g_{max} for grass is 3.7 mm s^{-1}. Note that when the species in the modelled area is are known, we suggest the g_{max} is selected accordingly. Here, we seek values that can represent the overall vegetation over the urban area in Beijing, and therefore the average is taken from different species.

Appendix F: Comparison of parameters for modelling domain with different radii

Table F1. Land surface fraction for modelling domain with different radii, where "Paved" denotes paved surface, "Bldgs" buildings, "EveTr" evergreen tree, "DecTr" deciduous tree, "Grass" grassland and lawn, "Bsoil" bare soil, "Water" water body.

	Radius (m)			
	500	750	1000	1500
Fr_Paved	0.39	0.32	0.46	0.46
Fr_Bldgs	0.18	0.21	0.24	0.24
Fr_EveTr	0.04	0.04	0.02	0.02
Fr_DecTr	0.18	0.18	0.11	0.01
Fr_Grass	0.20	0.24	0.16	0.17
Fr_Bsoil	0	0	0	0
Fr_Water	0.01	0.01	0.01	0.01
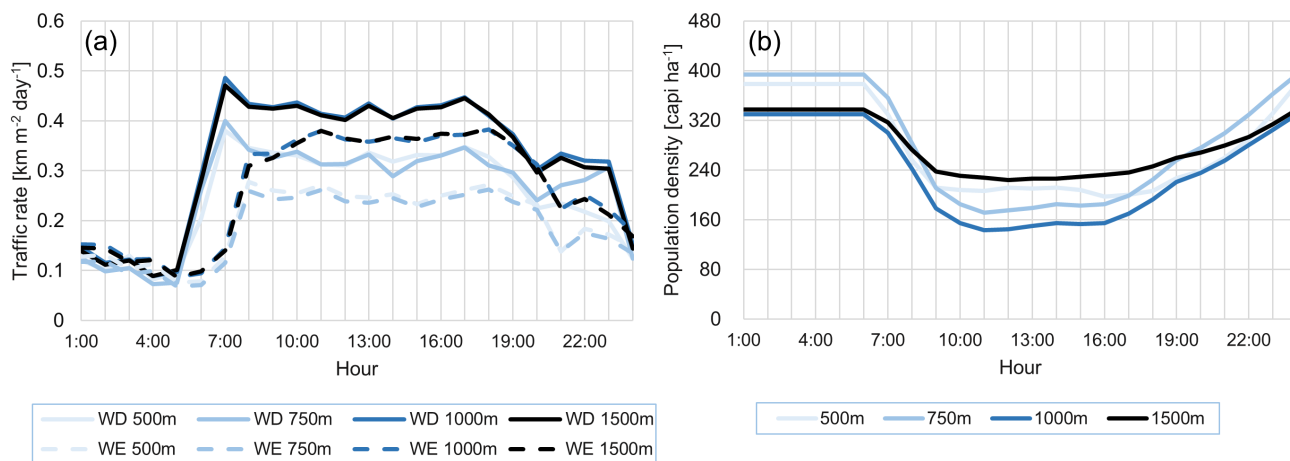
Figure F1. Diurnal cycles of (a) traffic rate and (b) population density for modelling domain with different radii, where WD denotes weekday and WE weekday.

Code and data availability. The data sets are openly available, including the complete model cases of SUEWS, the meteorological, radiation, and turbulent flux measurements, codes for LAI model optimization using CMA-ES, and codes to reproduce the statistics and figures (Zheng et al., 2022).

720 *Author contributions.* YZ, MH, HL and LJ conceptualized the study. YZ performed the SUEWS model cases, analyzed the results, and prepared the figures. HL, XC, YW, and JA collected the data. HSL performed the fitting of maximum photosynthetic rate. LJ and HL supervised the study. All authors contributed to writing and preparing the manuscript.

Competing interests. Leena Järvi is a member of the editorial board of Geoscientific Model Development. The peer-review process was guided by an independent editor, and the authors have also no other competing interests to declare.

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