Response to Referee #2

We thank both referees for their efforts and constructive comments. Each referee's comments are shown below in ***italics***, followed by our point-by-point responses in **blue** and relevant text in **red**.

Anonymous Referee #2

This paper proposes a new model for estimating biogenic carbon fluxes from urban areas. This model, called SMUrF uses a new global solar-induced fluorescence product (cSIF) and biome specific GPP-SIF relationships to create a temporally and spatially explicit flux product specifically turned for urban vegetation, which is notoriously difficult to model accurately. Respiration is also carefully considered in this new model, using a neural net approach. The paper does an excellent job of describing the intricate (and very numerous) processes involved and the model, and the result is a truly exciting work that is sure to be of great interest to the flux modelling community. Although the SMUrF model contains a large number of assumptions (as any model of this scope does), and will likely be refined in the future, the authors cleverly acknowledge that this version Discussion paper is only the first iteration of the SMUrF model by referring to this version as "v1" in the main title.

We appreciate the constructive feedback from the reviewer and have tried our best to improve the clarity of the text plus figures and redo the demonstration on analyzing column CO_2 observations.

The model relies on an assumption that GPP and SIF have a linear relationship, and that the slope of this relationship (alpha) is only a function of biome type. The plots for these calculations are buried in the supplemental, and for many of the biomes, the relationship does not appear to be linear. It is unclear if this non-linearity in addressed in the uncertainty analysis. This is the one part of the analysis that I wish was discussed in more detail.

We are aware of the non-linearity between GPP and SIF at finer temporal scales (e.g., sub-diurnal scales), suggested by a few studies analyzing the ground-based SIF and GPP measurements. The non-linearity results from the complex relationship between the light use efficiency (GPP / APAR) and the SIF yield (SIF / APAR) and its non-linear behavior under different light conditions. Although the

We added two discussions on the nonlinearity of GPP-SIF relationship in the methodology section (Sect. 2.5):

"It is worth noting that non-linearity in GPP and SIF has been reported under some circumstances, e.g., sub-diurnal scales or unstable light conditions (e.g., Yang et al., 2018, Miao et al., 2018). The uncertainties in assuming linear GPP-SIF relationships across biomes were not explicitly quantified but were implicitly accounted for as part of the total uncertainties quantified from the model-observation comparison."

as well as in the discussion section (Sect. 4.2):

"Second, GPP within SMUrF is currently estimated as a linear function of SIF, using a set of constant biome-specific linear slopes (α) without considering temporal or inter-site variations. The adoption of SIF has dramatically benefited and simplified the GPP calculation, as no extra satellite indices or impervious fractions need to be plugged in. However, previous research based on ground-based SIF measurements (Miao et al., 2018; Wohlfahrt et al., 2018; Yang et al., 2018) revealed the GPP-SIF relation deviated from linearity at the sub-diurnal scale, under unstable light conditions, or heat stress. While SIF and absorbed PAR are linearly related, the GPP-SIF relationship can deviate from linearity due to complex LUE:SIF yield relationships in light-saturating vs. light-limiting regimes (Miao et al., 2018). Thus, considering additional environmental factors related to the modeling of light use efficiency—e.g., relative humidity, cloudiness, and growth stage of crops, could improve the SIF-based GPP estimates (Yang et al., 2018). Although the nonlinear GPP-SIF relationship was not explicitly accounted for in this first iteration of SMUrF, our estimated flux uncertainties against dozens of flux tower sites implicitly account for the overall potential error associated with the linear assumption. Nevertheless, we anticipate future efforts to add more degree of freedoms in the estimate of GPP-SIF relation."

In an effort to relate the SMUrF model output to XCO_2 observations from OCO-2, the X-STILT transport model was used to generate total-column footprints. The assemblage of Boston area footprints shown in Figure 12a. shows a satellite overpass that occurred while the winds were out of the NNE along the flight track. The forward model results shown in Figure 12b seem ok, but the plots in 12b,c are confusing, because they are not XCO_2, they are the spatially explicit contributions to the XCO_2 concentrations for the satellite observations.

Figure 12c,d show the anthropogenic and biogenic contributions in ppm from each upwind grid cell with respect to the downwind XCO_2. As mentioned in the figure caption, we often referred to those anthropogenic and biogenic contributions as spatial $XCO_{2.ff}$ and $XCO_{2.bio}$. These spatial contributions have units of ppm and are further calculated from the product between X-STILT column footprint [ppm /(μmol m-2 s-1)] and upwind fluxes [μmol m-2 s-1]. The spatial sum of these contributions arrives at the total anthropogenic and biogenic anomalies at corresponding receptors, as shown in panel b).

The analysis in Figure 12e seems problematic, particularly for the treatment of the background concentration. The background value chosen appears somewhat arbitrary and taken from a region downwind of the city. The correlation between the binned OCO-3 observations (black triangles) and the full model result (purple line) is not particularly strong. The author states that the additional of SMUrF to the analysis is an improvement over just using a fossil fuel inventory, but other papers (such as the cited Sargent, 2018) spend a lot more time dealing with incorporating the biosphere with these types of transport models. While SMUrF represents an important step forward in assimilating SIF measurements into a biosphere carbon flux model, the STILT analysis at the end is incomplete, and, in my opinion, the paper would be better off for dropping this part entirely. Many researchers will surely be eager to explore the use of SMUrF with transport models to compare with satellite data, but these comparisons will need to spend a lot more time on dealing with subtleties such as determining the background. Because XCO_2 anomalies are so small over cities (typically a few ppm at most), a careful error analysis would also be needed, which is lacking here.

1) We agree with the reviewer's criticism - it might be too soon to conclude that using SMUrF can effectively improve the background along satellite swath, particularly given only one case examined. However, we hope to provide a demonstration of how SMUrF can be used with transport models and emphasis the role of urban-rural gradient in NEE and resultant biogenic XCO_2 signals played in the background definition. We feel that even though this is a model description paper, it is illustrative for the reader to see an application of the model in helping to interpret satellite XCO_2 data.

   To deemphasize the quantitative results from a limited number of analyses, we modified a relevant sentence in the Abstract to read.

   Initial text - "By examining a few summertime satellite tracks over four cities, we found that the urban-rural gradient in column CO_2 (XCO_2) anomalies due to NEE can sometimes reach ~0.5 ppm and be close to XCO_2 enhancements due to $FFCO_2$ emissions."

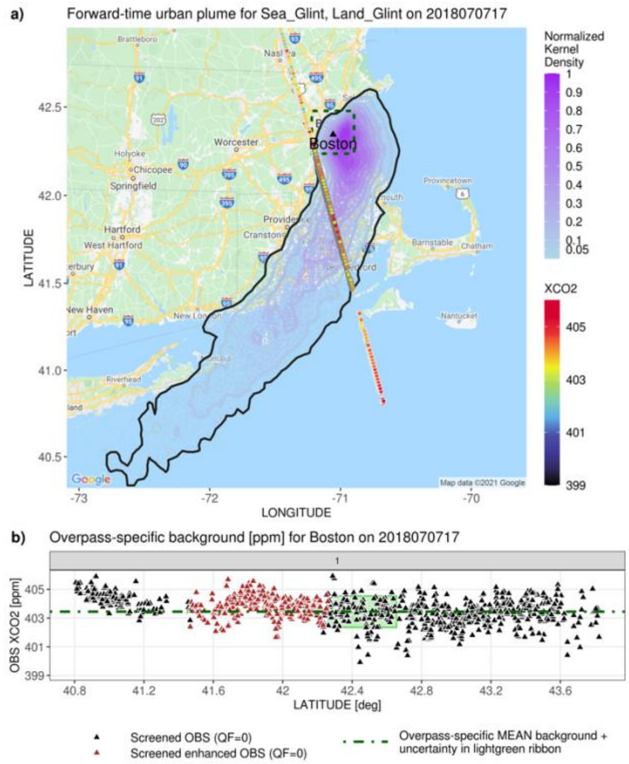
   Modified text - "To illustrate the application of SMUrF, we used it to interpret a few summertime satellite tracks over four cities and compared the urban-rural gradient in column CO_2 (XCO_2) anomalies due to NEE against XCO_2 enhancements due to $FFCO_2$ emissions."

2) In terms of the background definition, we agree that the initial choice can be arbitrary and calculating the proper background for column data is especially challenging and has been extensively investigated in our previous work (Wu et al., 2018, hereinafter Wu2018). **We now followed the overpass-specific approach illustrated in Wu2018, that is calculated from the average observed XCO_2 over the background latitude band.** The relevant figure regarding the overpass-specific approach has been added to the supplement as Fig. S13 in the revised manuscript.

Specifically, we leveraged the forward-mode of STILT where STILT particles were continuously released forward in time from a box around Boston for 12 hours. The border of the urban plume is defined by fitting a normalized 2D kernel density (purple contour in the **Fig. S13** to the right) to particle locations during the few minutes where OCO-2 overpass the city. The intersection of the urban plume and the satellite swath give rise to the urban-polluted latitude range (red triangles in panel b). Then the background latitude range (42.26 to 42.76°N, green ribbon in panel b) is chosen to the north of the urban-polluted range, given 1) the geometry between the swath orientation and the wind direction and 2) possible contamination from oceanic fluxes over the region to the south of the urban plume.

We arrived at both the mean background along with its uncertainty for this swath as shown in dotted-dashed green line and green ribbon, which have values of 403.37 +/- 1.03 ppm. The background uncertainty can also be used in error analyses and atmospheric inversions like those conducted in Wu2018.

Supplementary Figure S13. Overpass-specific background following Wu et al. (2018).



3) **Next, we explain the reason for using this overpass-specific background**:

Wu2018 has carefully invested three common methods with different complexity in estimating $XCO_{2.bg}$. The reviewer is welcomed to read over Sect. 2.3 and Sect. 3.3 in Wu2018 for full details. For the convenience, we summarized main messages as follows and adopted the relevant two figures from Wu2018 (Figure S8 and S12, also shown on the next page) for explanations:

M1. a "trajectory-endpoint" method is investigated by assigning CO_2 values extracted from global models (e.g., CarbonTracker, CT) to trajectory endpoints including simulating biospheric, oceanic, and prior components. This method has been widely used in Lagrangian-based modeling work including the cited Sargent et al., 2018. **However, most prior work only had to deal with CO_2 measurements within the PBL where huge CO_2 anomalies are caused by either anthropogenic or biogenic. When applying this trajectory-endpoint method solely relying on model simulations to interpreting column CO_2 measurements, this approach may often lead to potential "bias" in background values (orange lines in Figure S12 adopted from Wu2018).** Although there is hardly a "truth" for XCO_2 background, the modeled total XCO_2 based on this approach appears to be unreasonably higher or lower than the retrieved XCO_2 by 1-2 ppm (orange dotted-dashed line vs. black solid line in Figure S8 of Wu2018). These mismatches of 1-2 ppm can already be huge given small anthropogenic XCO_2 enhancements and is caused by potential uncertainties in the adopted global models (e.g., CT) with accumulated errors in the endpoint of STILT (further result from wind errors).

M3. an "overpass-specific" background as described earlier. **$XCO_{2.bg}$ calculated by combining observations and wind information from forward-mode of STILT can be more consistent with the retrieval and account for upwind-downwind geometry, which is better than approaches that solely rely on models OR observations. The biggest hurdle would be wind bias in STILT, which unfortunately can affect the M1 trajectory-endpoint background as well.**

The following Figure S12 and Figure S8 are adopted from Wu et al. (2018).

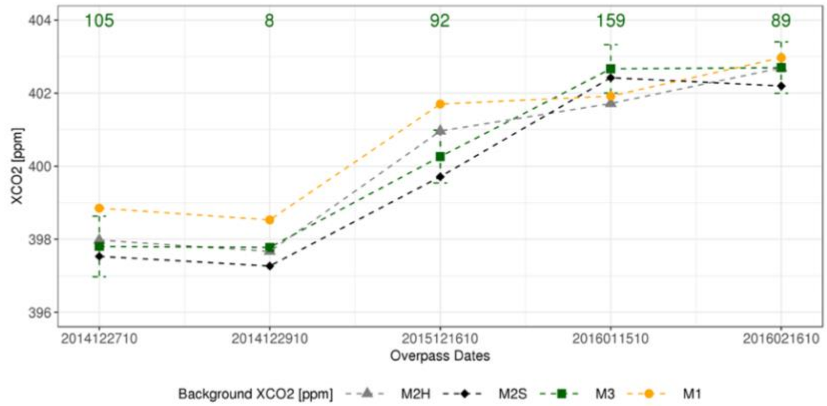


Figure S12. Same as **Fig. 6e**, except for using OCO-2 Lite b8. Numbers labeled in darkgreen donote the amount of screened soundings (QF = 0) using b8 in the background. Due to only 8 soundings for overpass on 2014122910, background uncertainty is hard to estimate (no error bar displayed).

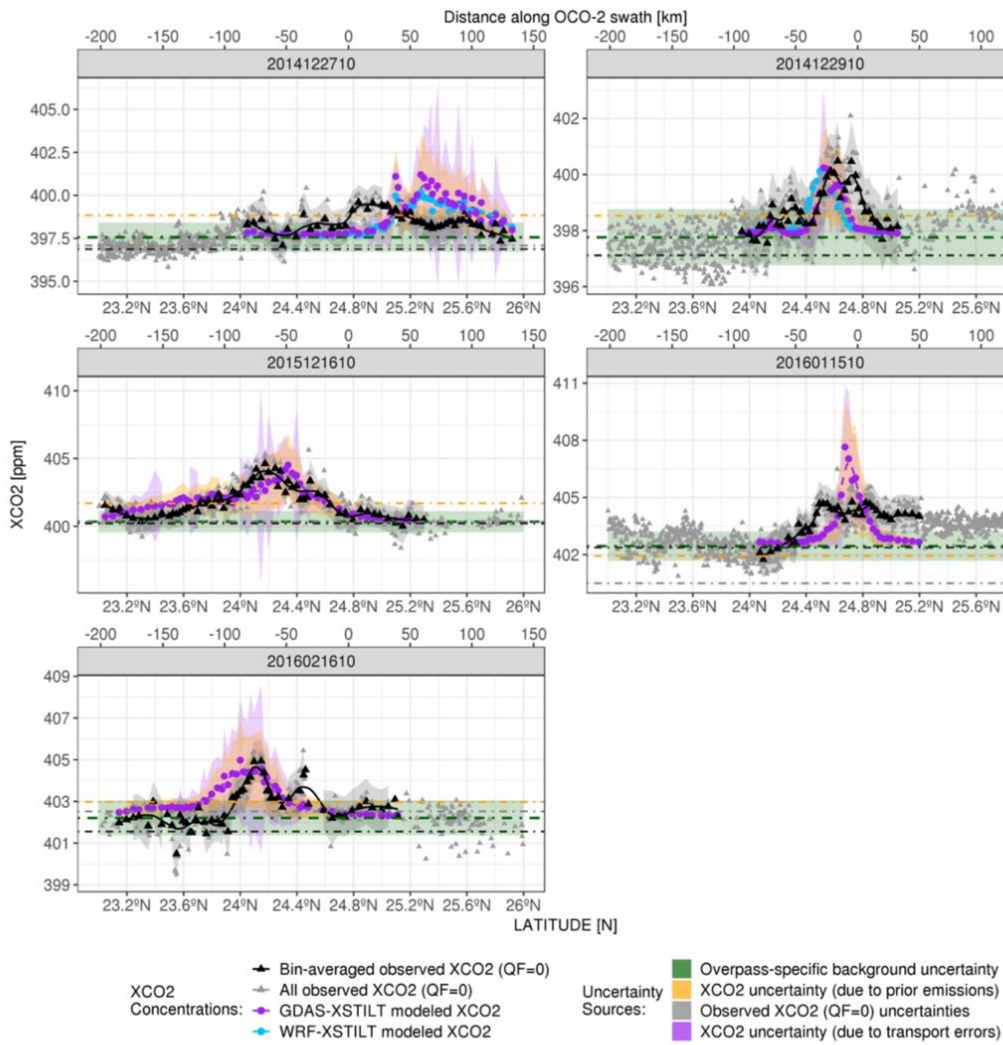
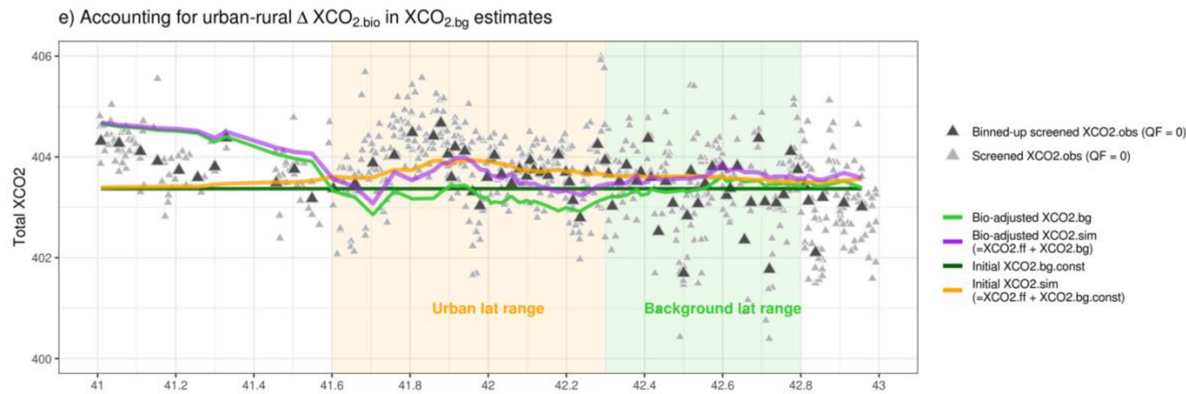


Figure S8. Same as **Fig. 8**, but for all five overpasses examined over Riyadh using OCO-2 Lite v7.

4) Lastly, we agree with the reviewer that the biogenic adjusted signal may not correlate strongly with the observations, possibly due to various reasons, e.g., 1) the bias in near-field wind direction, 2) uncertainties in both FF and biogenic fluxes, 3) retrieval error. We have now added a wind error analysis by comparing the modeled wind speed and directions against a NOAA radiosonde station (41.67N, 69.97W) adjacent to Boston city. Close to the overpass hour (07/07/2018 17 UTC), we see overall positive biases in the HRRR-based wind direction from the surface to 3 km. This positive bias potentially explains a northward modeled XCO_2 peak than the observed peak (latitude shift of about 0.1 degreeN in **Fig. 12e**).

time.string	u.bias	v.bias	ws.bias	wd.bias	rmse
07/07/2018 00 UTC	-2.29	-1.86	-1.36	16.6	3.08
07/07/2018 12 UTC	0.220	1.22	-1.70	2.68	1.91

Revised Figure 12e:



We may argue that if the aim of a study is to quantify FF emissions over cities surrounded by vegetations (e.g., Sargent et al., 2018), a comprehensive error analysis or even an atmospheric inversion is needed. In future work, we will follow the full error analysis and potentially a scaling factor type atmospheric inversion conducted in Wu2018 to make more quantitative results. However, given the already lengthy manuscript and the main scope of this work being model presentation, we simply modified the text in Sect 4.1 for clarifications.

"To facilitate visualization and understanding of $\Delta XCO_{2.bio}$ and bio-adjusted background, let us return to the Boston case again (**Fig. 12**). Following the "overpass-specific approach" proposed in Wu et al. (2018), we took the near-field wind direction into account and defined the background latitude range as 42.26°–42.76° N (light green ribbon in **Supplementary Fig. S13b** and **Fig. 12e**). The constant background is 403.37 ppm (dark green line in **Fig. 12e**) with an uncertainty of 1.03 ppm containing both the retrieval uncertainty and XCO_2 noise in the background range. The mean $XCO_{2.ff}$ and $XCO_{2.bio}$ anomalies within the background region are 0.23 ppm and –1.41 ppm, respectively. After integrating the bio-gradient $\Delta XCO_{2.bio}$, a new bio-adjusted background varies along latitude (light green line in **Fig. 12e**). If modeled $XCO_{2.ff}$ is added to the bio-adjusted background, the resultant total XCO_2 better reproduces the latitudinal variations of the measured mean values (**Fig. 12e**). Both the observed XCO_2 and modeled XCO_2 correcting for $\Delta XCO_{2.bio}$ exhibit dips in XCO_2 on both sides outside the urban peak, which is missing from the model result using the constant background (orange line in **Fig. 12e**).

A comprehensive error analysis is required in future work to draw quantitative conclusions from model-data XCO_2 comparisons given various uncertainty sources. For instance, the modeled XCO_2 appears to be broader latitudinally with a lower amplitude and a small latitude shift of around 0.1° compared to observed XCO_2 (purple line versus black triangles in **Fig 12e**) likely due to bias in wind speed and direction. Nonetheless, neglecting the latitudinal/spatial gradient in biogenic XCO_2 anomalies given gradients in NEE affects the extracted urban signal and the inferred $FFCO_2$ emissions in this case."

We also reemphasis the future needs in Sect. 4.2 and deemphasis the quantitative conclusion in the abstract (as mentioned in above point 1):

> "We also hope to examine more cities and different times of the day in future studies to better study the relative biogenic and anthropogenic contributions to XCO_2 anomalies. And, incorporating uncertainties in biogenic fluxes and resultant $XCO_{2.bio}$ is needed for future studies with aims of understanding urban signals especially over the growing seasons."

In summary, we clarify the key point in this manuscript being the urban-rural gradient in biogenic fluxes and CO_2 anomalies. Even though one may not follow the same exact constant background approach with biogenic adjustments as we showed in Sect. 4.1, one needs to consider the urban-rural contrast in biogenic fluxes that is lacking in many XCO_2-based studies.

The manuscript contains a large number of figures, many with numerous subplots. While this isn't uncommon for GMD papers describing a new model, this particular work would benefit from slimming down some of the figures. I've discussed a few of the figures individually below:

We appreciate these individual comments and have made some rearrangements to the figures.

Figure 1: This is a really well laid out flow chart. It took me a while to get through it all, but it was really helpful in understanding the model, and I like how it was labeled with section and figure references.

We thank the reviewer for the recognition and are very glad this flow chart worked well in the end.

Figure 2: Subplot c needs units for alpha values. Also, subplots are not labeled.

We have now added the unit for α values in the figure caption, i.e., (umol m^{-2} s^{-1}) / (mW m^{-2} nm^{-1} sr^{-1}).

Figure 6: This figure is way too complicated. In addition to their being too many cities, I can't easily discern what the take home message is supposed to be from all of these plots.

We may argue that this zoom-in-and-out panel plot gives a nice overview of 1) anthropogenic and biogenic CO_2 fluxes from urban center to its surrounding and 2) how regional total CO_2 fluxes vary with seasons. One can spot the urban hotspots where anthropogenic CO_2 "beat" down the biogenic CO_2 fluxes.

Figure 7: Again, too many subplots. It would be easier to read if thier were fewer cities selected. To me, the interesting information in this figure is both the magnitude of max NEE for different cities and the timing of when that max NEE occurs. Perhaps it would be more impactful to show a different type of plot. Perhaps a scatter plot with the x-axis being day-of-year for the NEE peak and the y-axis being peak magnitude? You could then pack a bunch more cities into one plot, and label the cities in the scatterplot.

We appreciate the suggestions from the reviewer but may argue that the current presentation can provide a broad view for cities across multiple continents and hopefully facilitate readers with different cities of interests.

Figure 8: These time of day plots are nice, but the half-circle makers are hard to see.

We have now replaced circles with solid dots.

Figure 10: Again, too many panels.

We have now moved two of the initial six panels to the supplement (now as Fig. S12).

Figure 11: This is great. I wish there was more urbanVPRM comparisons with other cities. A real test of the usefulness of SMUrF is its performance compared to other models, especially those also tailored for urban areas.

Yes – we also wish to provide more model comparisons with other observations and model products for more locations, which require additional support and collaboration from data providers/users in the field.

Overall, this is an impressive manuscript. The model described is sure to make an impact in the community, and I know that I and other researchers look forward to working with it.

We thank the support from the reviewer and will keep improving the SMUrF model, given increasing understanding towards SIF, respiration, and urban biosphere as well as the availability of upcoming remote sensing data.

Specific line-by-line comments (mostly grammar stuff) are below:

p.6 L3 Grammar (". . .by trained on. . .")

Corrected – changed 'by trained on' to 'that trained on'

p.6 L10 "Laser" capitalized

Corrected – "Laser" to "laser".

p.6 L12 punctuation

We've modified this sentence as "AGB and its grid-level uncertainty [tons ha^{-1}] by definition describe the "oven-dry weight of the…".

p.6 L28 Underline on part of "(Sect. 3.2)."
p.13 L34 "than" -> "rather than"

Corrected.

p.14 L26 Why? Please add a sentence of explanation.

The point where NEE becomes negative is the number we read from Figure 3A3 and 3B3 in Hardiman et al. 2017 (also attached on the bottom right). They show that the NEE turned negative at ~5 am local time in July 2013. We extract SMUrF fluxes from the similar Boston area considered in Hardiman2017 and calculated the monthly mean diurnal cycle with the same flux unit (see figure below). It seems that the R_{eco} magnitude with its daily cycle as well as the maximum GPP between two models are almost identical. However, urbanVPRM GEE starts to become negative way earlier than SMUrF GEE, leading to an earlier turning point for net biospheric uptake (~5 am in urbanVPRM vs. 6-7 am in SMUrF). We have now modified this sentence as follows:

"In Boston, SMUrF reported similar NEE magnitude but with an hour delay where NEE becomes negative compared to urbanVPRM (**Supplementary Fig. S9** vs. Figure 3B3 in Hardiman et al., 2017), likely due to discrepancies in the hourly data that drive two sets of hourly GEE fluxes."

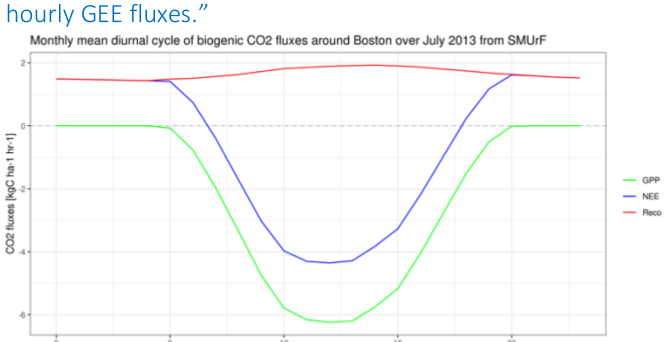


Figure S9. Monthly mean diurnal cycle of biogenic CO2 fluxes around the similar area considered in Hardiman et al. (2017).

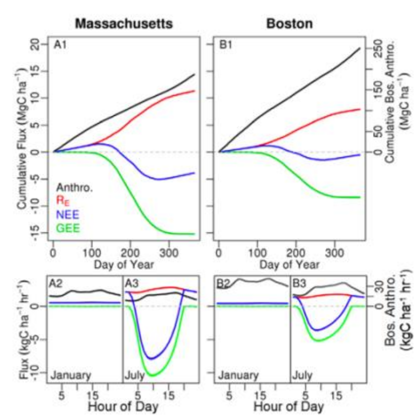


Fig. 3. Cumulative C fluxes (MgC ha^{-1}) for 2013 indicate that MA is a net biogenic C sink and that on an area-basis statewide anthropogenic emissions are of similar magnitude as biogenic fluxes (A1). Both biogenic and anthropogenic fluxes (kgC ha^{-1} h^{-1}) follow daily cycles, the amplitude of which varies seasonally (A2, A3). Boston's biogenic fluxes are dwarfed by anthropogenic C emissions (B1) but follow similar patterns as seen at the state-level (B1, B2). Anthropogenic fluxes in all B panels are plotted on a second y-axis to facilitate comparison with biogenic fluxes.

Figure adopted from Hardiman et al., 2017

p.15 L12 "prediction" -> "predictions"
p.15 L13 "as" -> "of"
p.15 L19 "amount" -> "amounts"
p.16 L15 "comparison" -> "comparisons"
p.16 L15 "insights on" -> "insight into"
p.16 L25 "turns" -> "turn"
p.16 L26 "GPP," -> "GPP as well as"

All corrected.

p.16 L31 Confusing sentence, please rewrite.

We have rewritten the relevant sentence: "Model discrepancies in producing R_{eco} lead to an overall higher R_{eco} and more positive NEE in SMUrF compared to urbanVPRM over LA (3rd column in **Fig. 11a**)."

p.16 L32 "grids" -> "gridcells"
p.17 L11 "examine" -> "examined"
p.18 L25 "how" -> "how a"
p.18 L25 "bio-gradient" -> "gradient"
p.20 L6 "on-board" -> "onboard"
p.20 L28 "10" in "Q10" shouldn't be italicized

All corrected. We thank the referee #2 for pointing all these grammatical issues out.