Supplementary information for

## Uncertainties in OCO-2 satellite retrievals of XCO<sub>2</sub> limit diagnosis of transport model simulation uncertainty

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**Figure S1:** Spatial location of 50 surface CO<sub>2</sub> concentration measurement sites across globe used in the MIROC4-ACTM inversion.



**Figure S2:** MIROC4-ACTM model simulated and ATom (a) concentration (b) difference CO<sub>2</sub> vertical profile, averaged over every 500 meters at every 5 latitudinal bands. FG and InvFG represents the prior and posterior concentration of the MIROC4-ACTM respectively. Full access to the gif file can be found here: https://zenodo.org/records/14504067



**Figure S3:** Time series of MIROC4-ACTM simulated and observed CO<sub>2</sub> concentration (ppm) at MLO (19.53 N, 155.57 W), and SYO (69.01 S, 35.59 W)



**Figure S4:** Scatter plot of MIROC4-ACTM model simulated CO<sub>2</sub> against CO<sub>2</sub> measured at different ATom-1; panel (a), ATom-2; panel (b), ATom-3; panel (c), ATom-4; panel (d) campaigns with colours delineating latitudinal locations.



**Figure S5:** XCO<sub>2</sub> difference between MIROC4- ACTM simulated XCO<sub>2</sub> against TCCON XCO<sub>2</sub> at 21 TCCON sites across the globe. " $\mu$ " and " $\sigma$ " represents the time series mean and 1 $\sigma$ -STDEVs of the XCO<sub>2</sub> difference.



**Figure S6:** Time vs latitude distribution of XCO<sub>2</sub> difference between InvFG and OCO–2 considering mean across global longitude for Land (panel–a), Ocean (panel–b), and Globe (Land + Ocean) (panel–c).



**Figure S7:** Location of individual surface  $CO_2$  measurements sites around the globe having measurements during OCO-2 measurement period with 90% availability for the same.



**Figure S8:** Specific sites aircraft measurements sampling information. (a) Number of data points in each altitude bins of 1000 meters. (b) Spatial sampling location of individual aircrafts with sampling altitude. Full access to the gif file can be found here: <u>https://zenodo.org/records/14504067</u>



**Figure S9:** Campaign aircraft measurements sampling information. (a) Number of data points in each altitude bins of 1000 meters. (b) Number of data points in each latitude bins of 30 degrees. (c) Spatial sampling location of individual aircrafts with sampling altitude. Full access to the gif file can be found here: https://zenodo.org/records/14504067



**Figure S10:** Vertical cross-section of  $CO_2$  difference between MIROC4-ACTM model simulated  $CO_2$  and observation from each ATom campaigns, ATom-1; panel (a), ATom-2; panel (b), ATom-3; panel (c), and ATom-4; panel (d) across global latitude taking mean every 2.5 degree latitude bin and 500 meter vertical height bin.



**Figure S11:** (a) TCCON sites across the globe situated at different location considering only sites having measurements during OCO-2 measurement period. (b) MIROC4-ACTM and TCCON  $XCO_2$  difference at different latitude across the globe. Here, y-ticks are representing TCCON stations names arranged in lower to higher latitude stations.



**Figure S12:** MIROC4-ACTM model simulated Land (black) and ocean (blue)  $CO_2$  flux for ATom-1 (first panel), ATom-2 (second panel), ATom-3 (third panel), and ATom-4 (last panel) denoted by campaigns for each track components over North America and neighbors, Pacific, Southern Ocean, and Atlantic specified with name in panel header in first panel averaged over the track. The bottom (top) x-axis in each panel represents land (ocean)  $CO_2$  flux.



**Figure S13:** (a) Sampling track traversed during the ATom-1 campaign. (b) Spatial model-observation  $XCO_2$  difference against OCO-2 over ATom-1 track during campaign. (c) , (d), (e), and (f) show model-observation  $CO_2$  difference over different tropospheric layers from vertical  $CO_2$  profile measurements of ATom-1 and  $XCO_2$  from OCO-2 for North America and neighbors, Southern Ocean, Pacific, and Atlantic segments respectively. Tropospheric layers are LT (light red), MT (orange), UT (dodger blue) and Total Column (teal), and  $XCO_2$  (black) representation for difference against OCO-2. The first and second numbers on the right side of each middle and bottom panel represent the mean and 1- $\sigma$  standard deviation (STDEV) of model-observation difference across latitude or longitude respectively. In panel (d), due to less number of pixels present in Model-OCO-2, we have ignored longitude vs  $XCO_2$  bias.



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**Figure S16:** (a) Sampling track traversed during ATom-4 campaign. (b) Spatial model-observation  $XCO_2$  difference against OCO-2 over ATom-4 track during campaign. (c) , (d), (e), and (f) shows model-observation  $CO_2$  difference over different tropospheric layers from vertical  $CO_2$  profile measurements of ATom-4 and  $XCO_2$  from OCO-2 for North America and neighbours, Southern Ocean, Pacific, and Atlantic segments respectively. Tropospheric layers are LT (light red), MT (orange), UT (dodger blue) and Total Column (teal), and  $XCO_2$  (black) representation for difference against OCO-2. The first and second number on the right side of each middle and bottom panel represents the mean and 1- $\sigma$  standard deviation (STDEV) of model-observation difference across latitude or longitude respectively.



**Figure S17:** Model simulated concentration (x-axis) and observed concentration (y-axis) associated with vertical CO<sub>2</sub> profile for all aircraft sites SAN, TEF, RBA, and ALF. The line is best fit linear regression line between the dataset and numbers, "r" and "p" are represents correlation and significance levels.