SUPPORTING INFORMATION

Photochemical Model Assessment of Single Source NO_2 and O_3 Plumes Using Field Study Data

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Table S-1. Models and source attribution options used for each case study. The grid resolution is also noted for each combination of model and source attribution approach.

Case Study	Brute-Force Sensitivity	Source Apportionment	DDM
Hopewell	CMAQ 12, 4, 2, and 1 km	CMAQ ISAM option 1, 2, 3, 4, and 5 at 2 km	CMAQ 2 km
	CAMx 2 km	CAMx OSAT and APCA at 2 km	
TVA	CMAQ 2 km	CMAQ ISAM option 1, 2, 3, 4, and 5 at 2 km	CMAQ 2 km
	CAMx 2 km	CAMx OSAT and APCA at 2 km	
Edgewater	CMAQ 4, 2, and 1 km		

Table S-2. A description of the various ISAM options available in the CMAQ model. Option 5 was a combination of option 2 for NO_2 limited conditions and option 4 for VOC limited conditions. This table also includes species used to influence source attribution for each option.

```
INTEGER :: ISAM_SPC_BIAS = 2          ! which chemistry are biased in apportioning reaction yields
                                      ! to source reactant
                                      ! 1 for none so divided equally between sources' reactant
                                      ! 2 for all products apportioned to sources with NO, NO2, NO3, HONO, ANO3
                                      !    -equally if reactants are neither or both
                                      ! 3 for all products apportioned to sources with Case 2 plus HCHO, CH3CHO,
                                      ! Acetone, Lumped Ketones, Isoprene peroxy radical, acetyl peroxy radical and peroxy
                                      ! radical operators (XO2 and XO2H)
                                      !    -equally if reactants are neither or both
                                      ! 4 for all products apportioned to sources with HCHO, CH3CHO,
                                      ! Acetone, Lumped Ketones, Isoprene peroxy radical, acetyl peroxy radicals and peroxy
                                      ! radical operators (XO2 and XO2H)
                                      !    -equally if reactants are neither or both
                                      ! 5 to switch between Cases 2 and 3 based on whether
                                      ! production H2O2 over production HNO3 less than VOC_NOX_TRANS that
                                      ! has default value of 0.35
REAL :: VOC_NOX_TRANS = 0.35          ! H2O2 to HNO3 marking transition from NOx to VOC limiting O3 production
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                                      Option 1, Option 2, Option 3, Option 4,            Option 5
NO,                                       NO,      YES,     YES,       NO,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){YES}else{YES}
NO2,                                      NO,      YES,     YES,       NO,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){YES}else{YES}
NO3,                                      NO,      YES,     YES,       NO,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){YES}else{YES}
HONO,                                     NO,      YES,     YES,       NO,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){YES}else{YES}
ANO3[i,j],                                NO,      YES,     YES,       NO,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){YES}else{YES}
HCHO,                                     NO,       NO,     YES,      YES,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){ NO}else{YES}
CH3CHO,                                   NO,       NO,     YES,      YES,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){ NO}else{YES}
Acetone,                                  NO,       NO,     YES,      YES,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){ NO}else{YES}
Lumped Ketones,                           NO,       NO,     YES,      YES,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){ NO}else{YES}
Isoprene peroxy radical,                  NO,       NO,     YES,      YES,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){ NO}else{YES}
Acetyl peroxy radicals,                   NO,       NO,     YES,      YES,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){ NO}else{YES}
peroxy operators (XO2 and XO2H),          NO,       NO,     YES,      YES,    IF( PH2O2/PHNO3 > VOC_NOX_TRANS){ NO}else{YES}
```

Table S-3. Aggregated model performance metrics for chemically speciated $PM_{2.5}$ components made as part of the Chemical Speciation Network (CSN).

Specie	Network	N	Mean Bias ($\mu g/m^3$)	Mean Error ($\mu g/m^3$)	Normalized Mean Bias (%)	Normalized Mean Error (%)	r^2
PM2.5 sulfate ion	CSN	9	-0.30	0.36	-26.08	31.66	0.86
PM2.5 nitrate ion	CSN	9	-0.14	0.14	-88.61	88.61	0.67
PM2.5 elemental carbon	CSN	9	-0.11	0.13	-29.16	33.07	0.26
PM2.5 organic carbon	CSN	9	0.41	0.52	15.72	19.95	0.87
PM2.5 ammonium ion	CSN	9	-0.02	0.09	-9.63	35.69	0.83

Table S-4. Aggregated model performance metrics for MDA8 O_3 for all model-observed pairs, a subset where modeled values exceed 60 ppb, and a subset where observed values exceed 60 ppb.

Specie	Network	N	Mean Bias (ppb)	Mean Error (ppb)	Normalized Mean Bias (%)	Normalized Mean Error (%)	r^2
MDA8O3	AIRS - ALL	385	7.12	7.68	15.58	16.80	0.65
MDA8O3	AIRS - Model > 60 ppb	68	7.81	8.71	13.81	15.40	0.15
MDA8O3	AIRS - Obs. > 60 ppb	23	-0.63	4.05	-0.96	6.22	0.21

Figure S1. Map of area around Hopewell, Virginia, USA. Orange sources were included in the Hopewell complex. The VCU pandora location is also shown.

Figure S2. Modeled and measured O_3 and NO_2 in a plume downwind of the TVA Cumberland power plant during July 1999. Model predictions are shown for CAMx brute-force difference (zero-out) and each option in the CAMx source apportionment approach (OSAT and APCA).

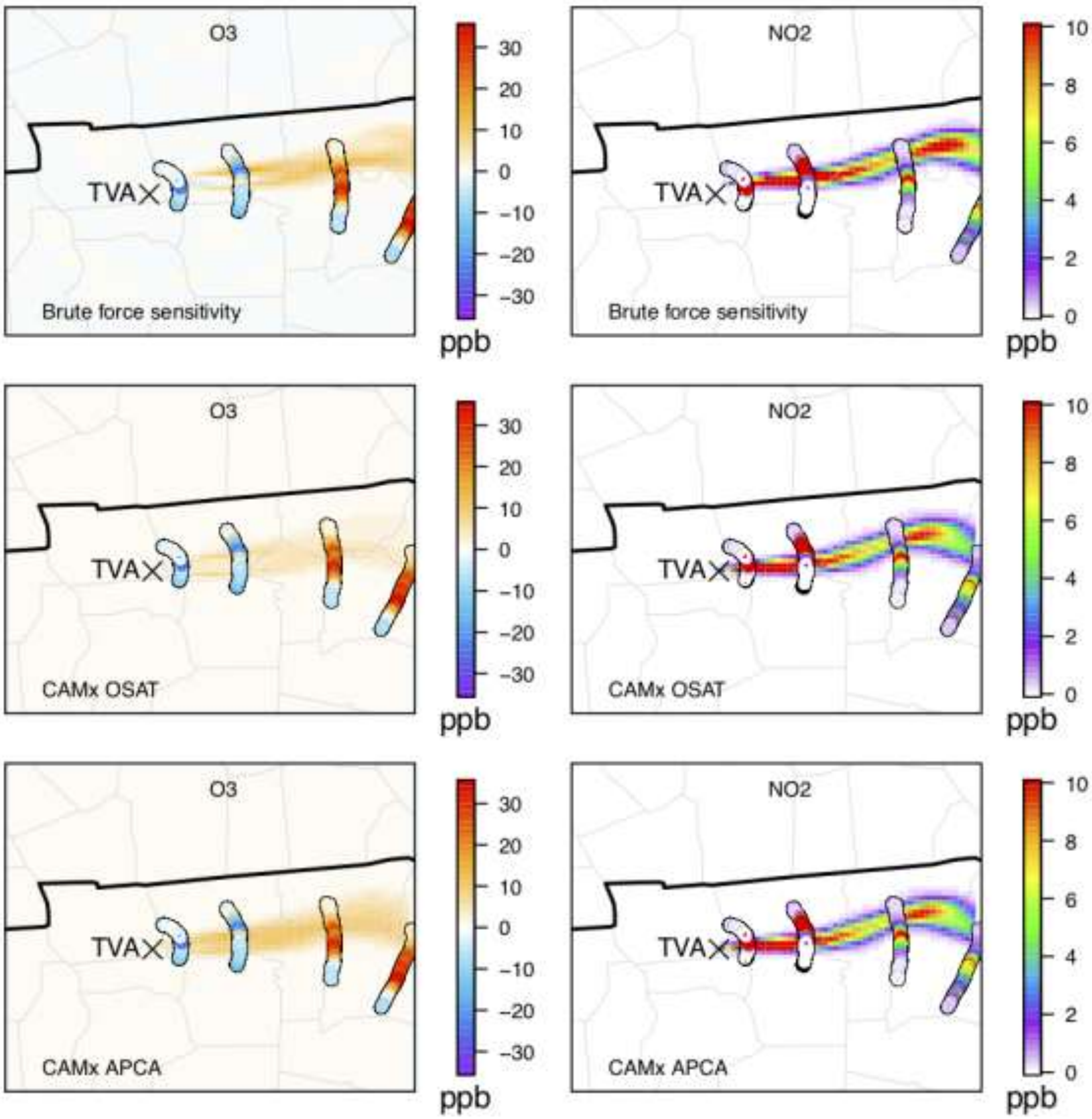

Figure S3. Aircraft altitude and distance from Hopewell for the July 19 and 20, 2017 flights.

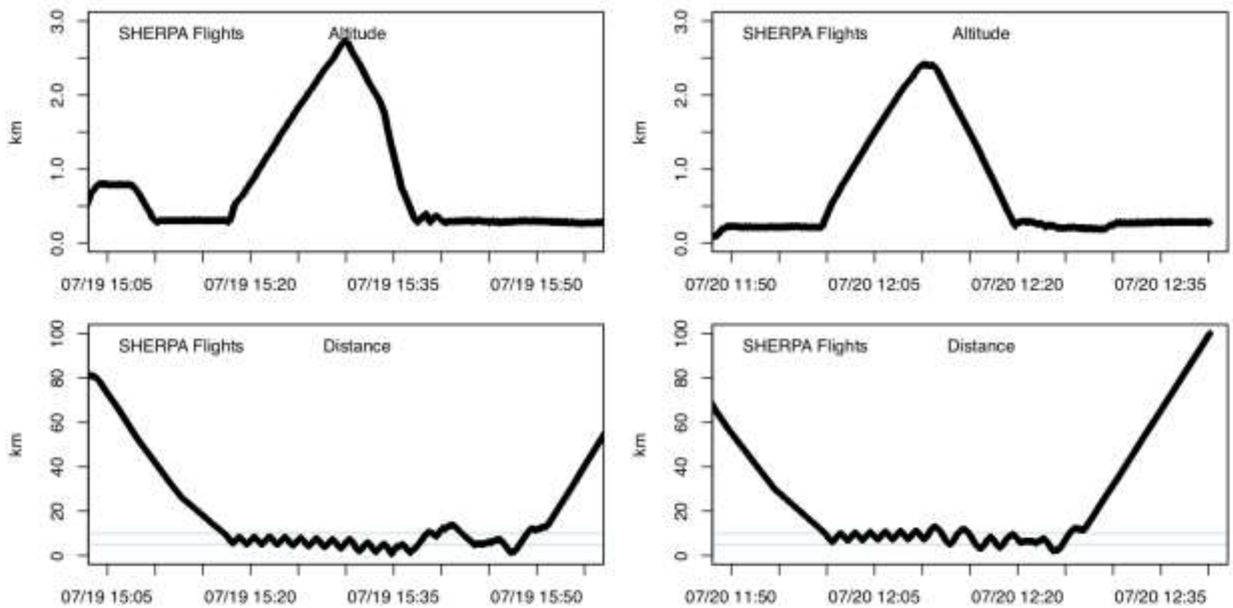

Figure S4. Daily prediction-observation pairs for speciated $PM_{2.5}$ components and MDA8 O_3. Model predictions were extracted from the CMAQ 2 km simulation.

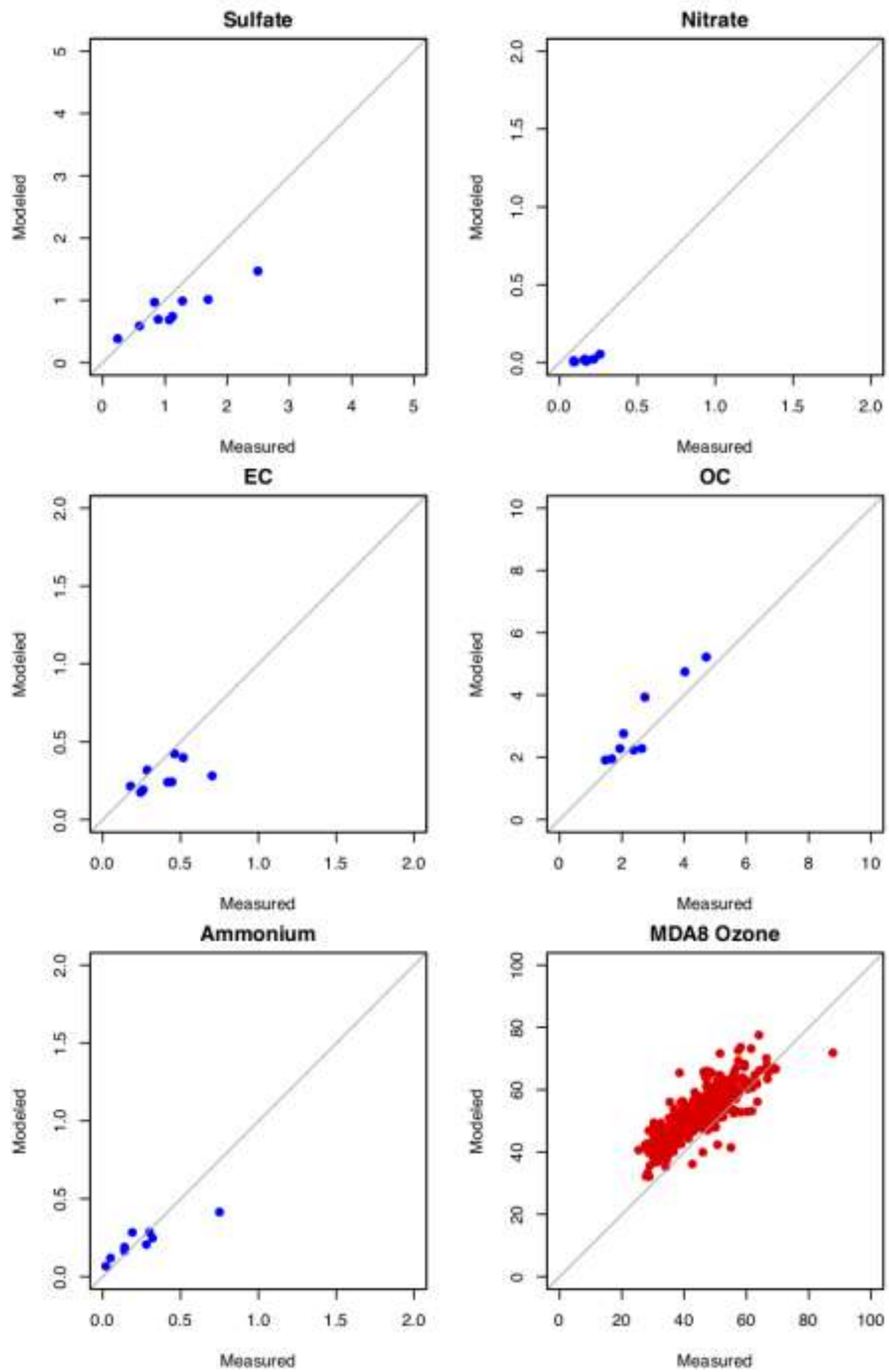

Figure S5. July 2017 episode average surface level 2 km modeled (CMAQ) primary and secondary pollutant impacts from Hopewell.

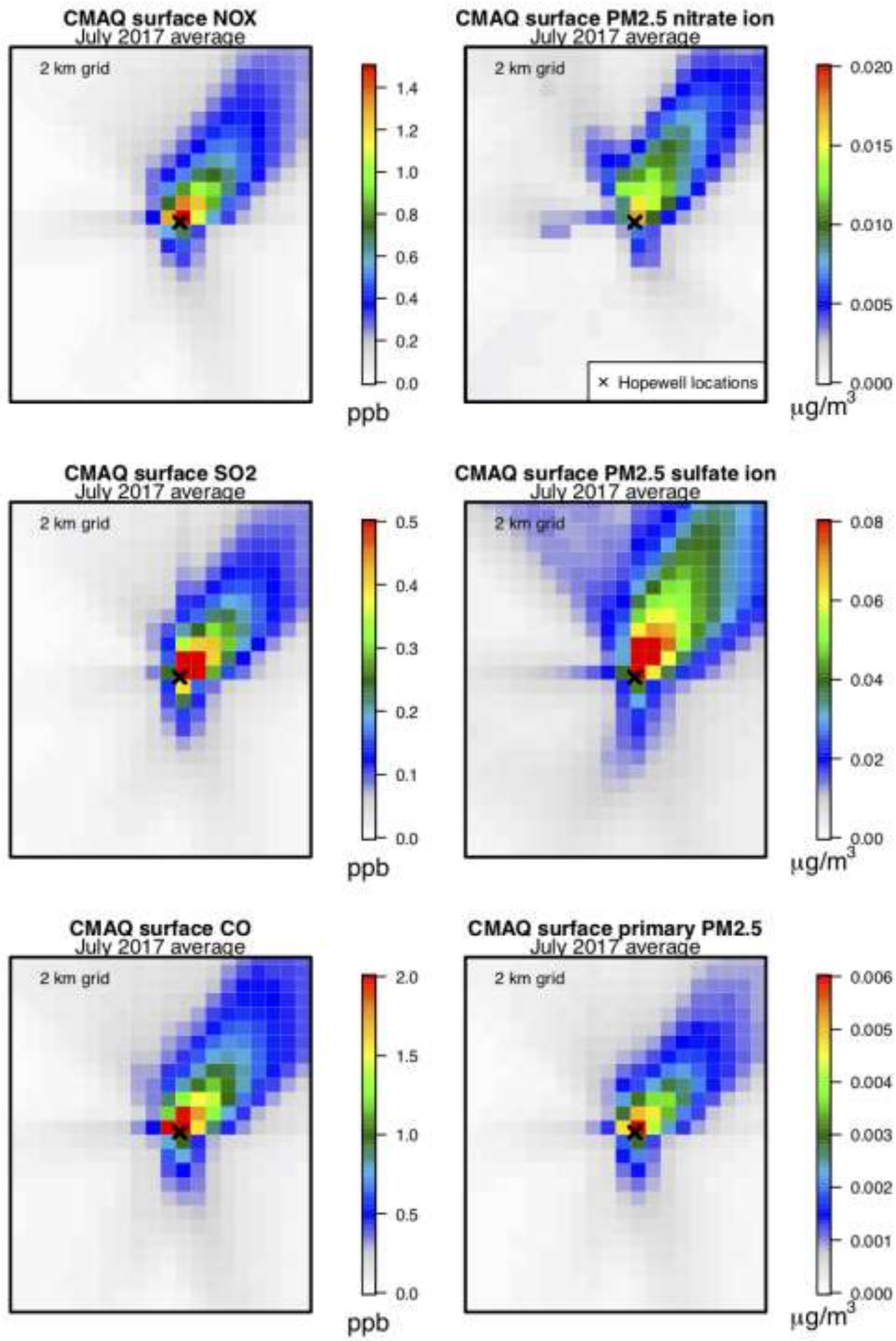

Figure S6. July 2017 episode average surface level 4 km modeled (CMAQ) primary and secondary pollutant impacts from Hopewell.

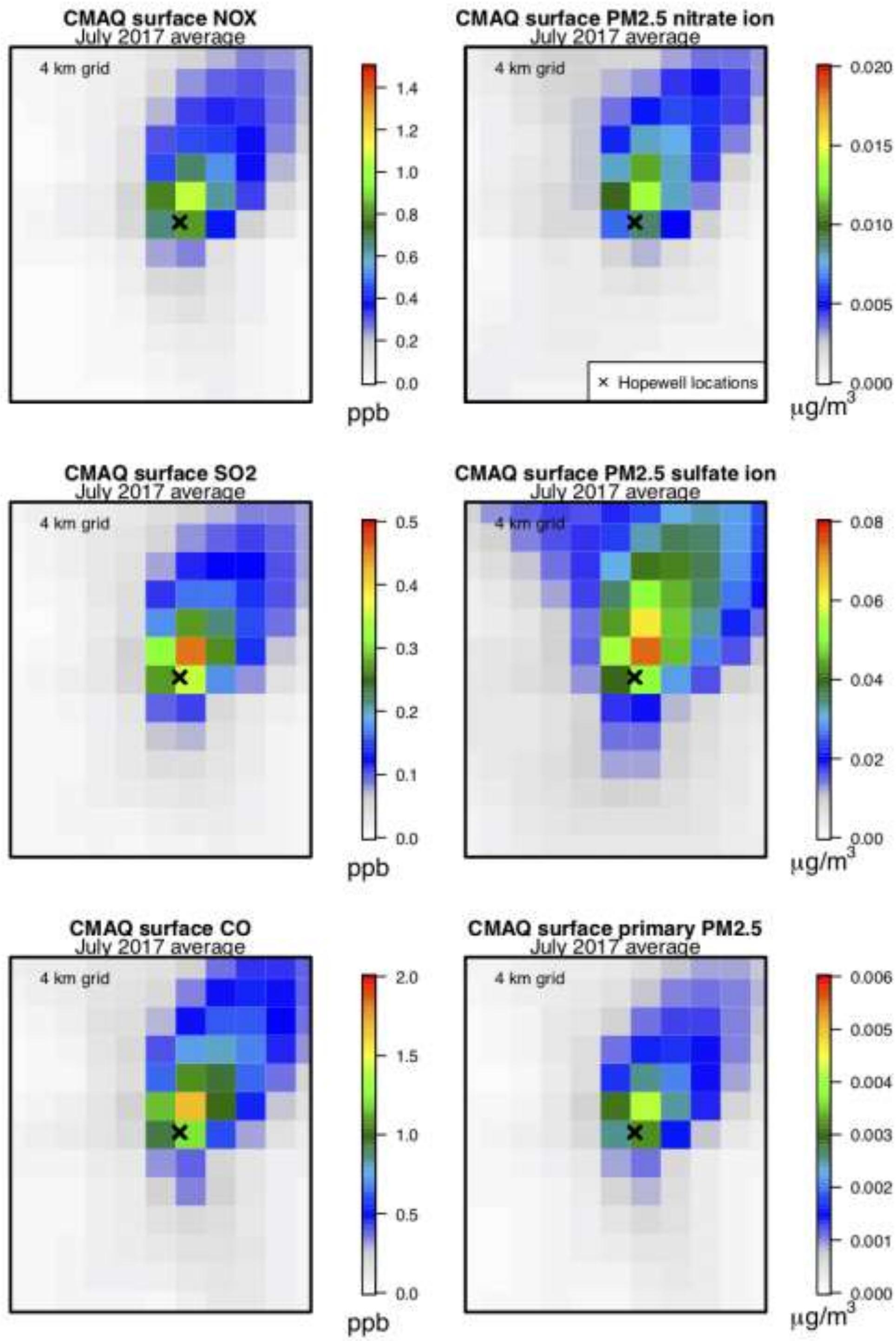

Figure S7. July 2017 episode average surface level 12 km modeled (CMAQ) primary and secondary pollutant impacts from Hopewell.

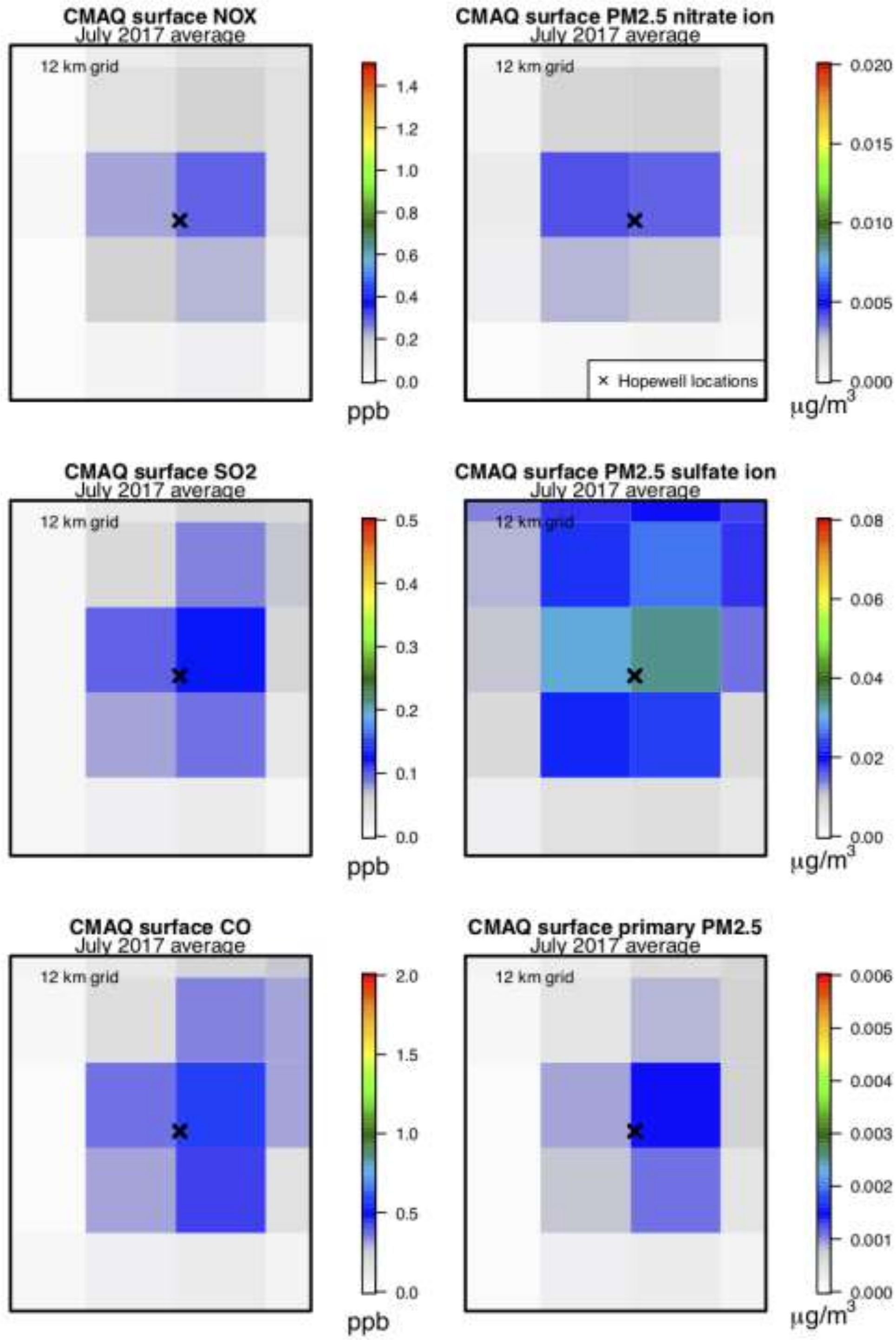

Figure S8. CMAQ 2 km (top panels) ISAM model OPTION 1 predicted surface level NO_X at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

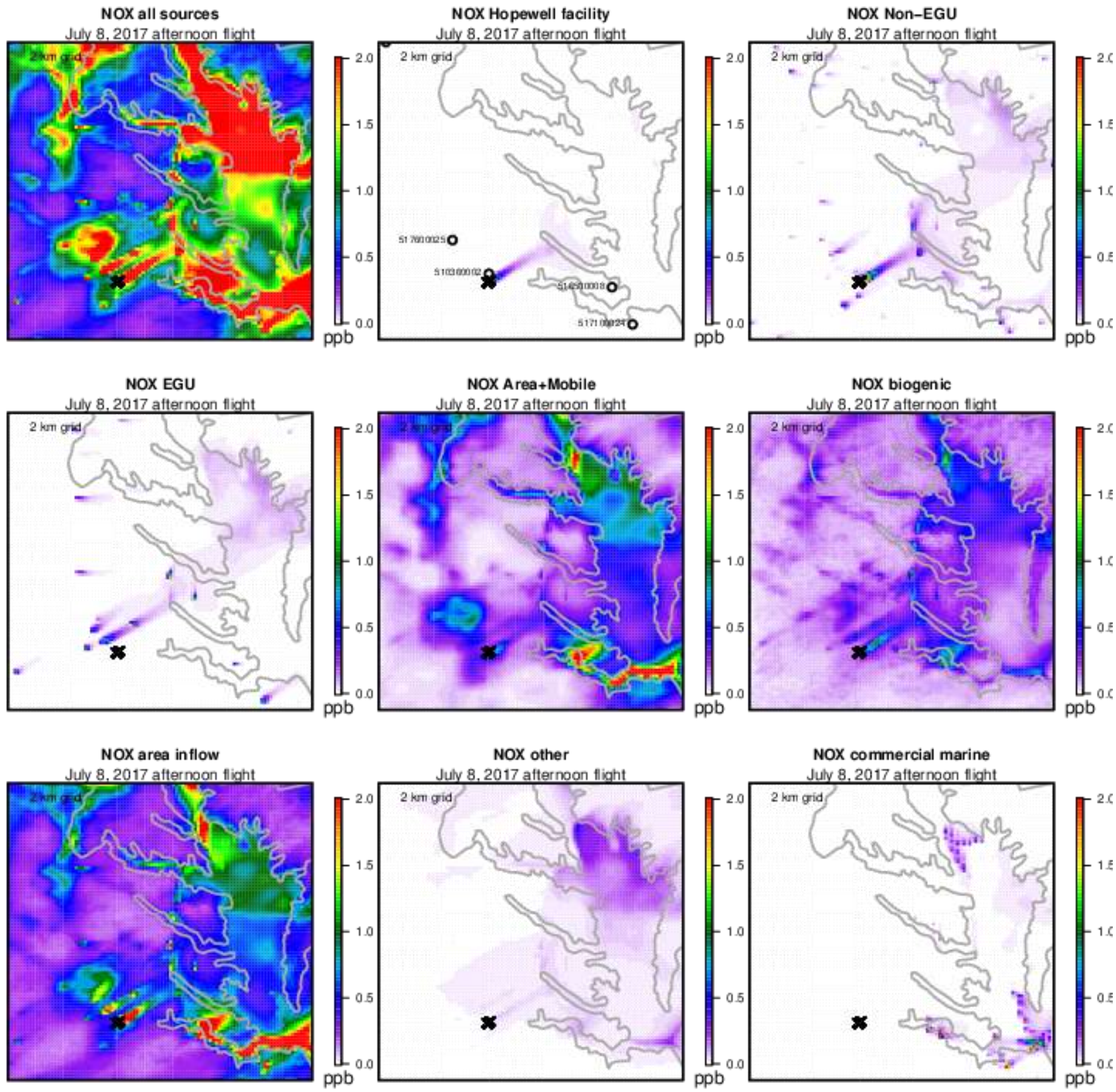

Figure S9. CMAQ 2 km (top panels) ISAM model OPTION 2 predicted surface level NO_X at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

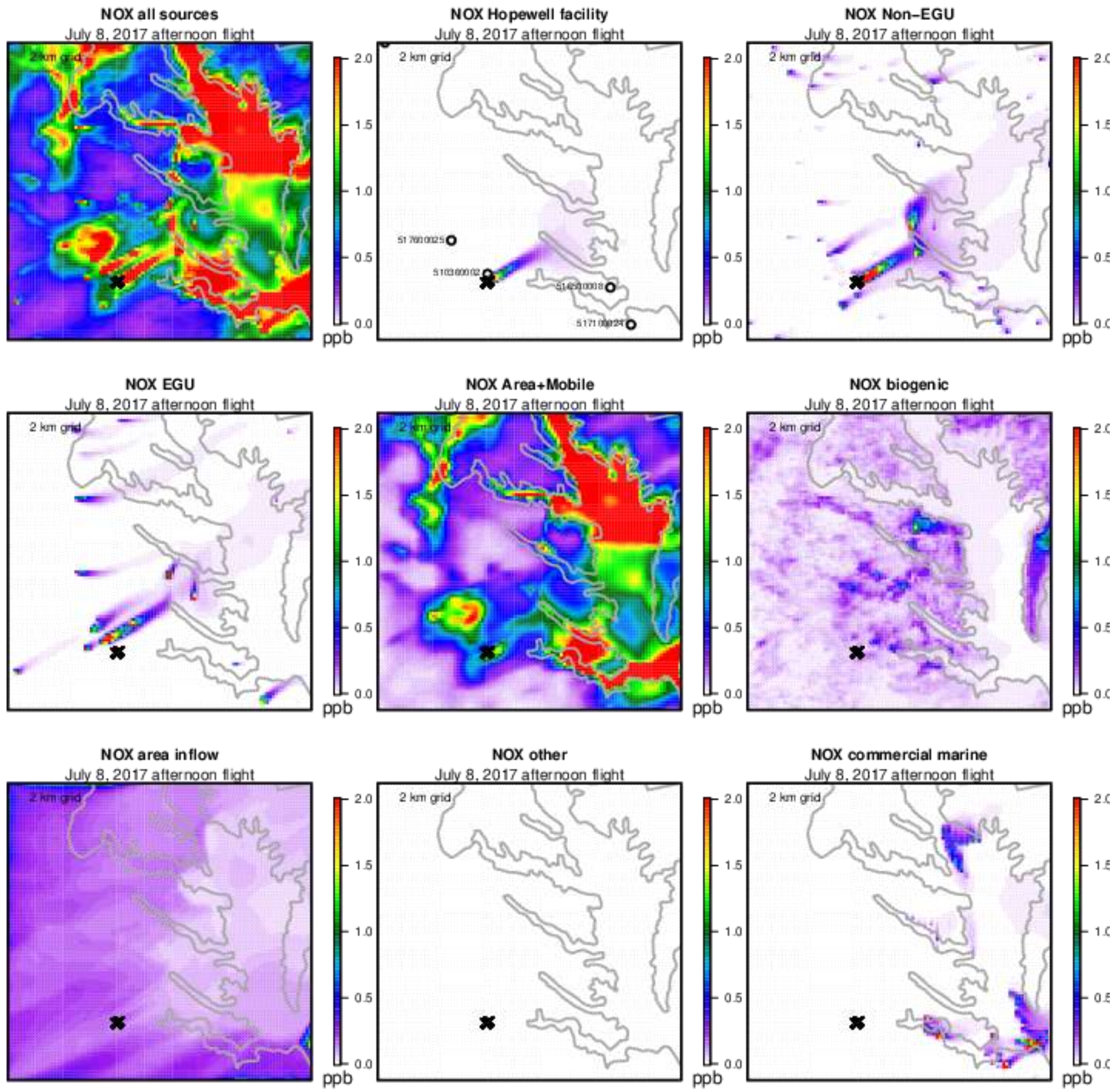

Figure S10. CMAQ 2 km (top panels) ISAM model OPTION 3 predicted surface level NO_X at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

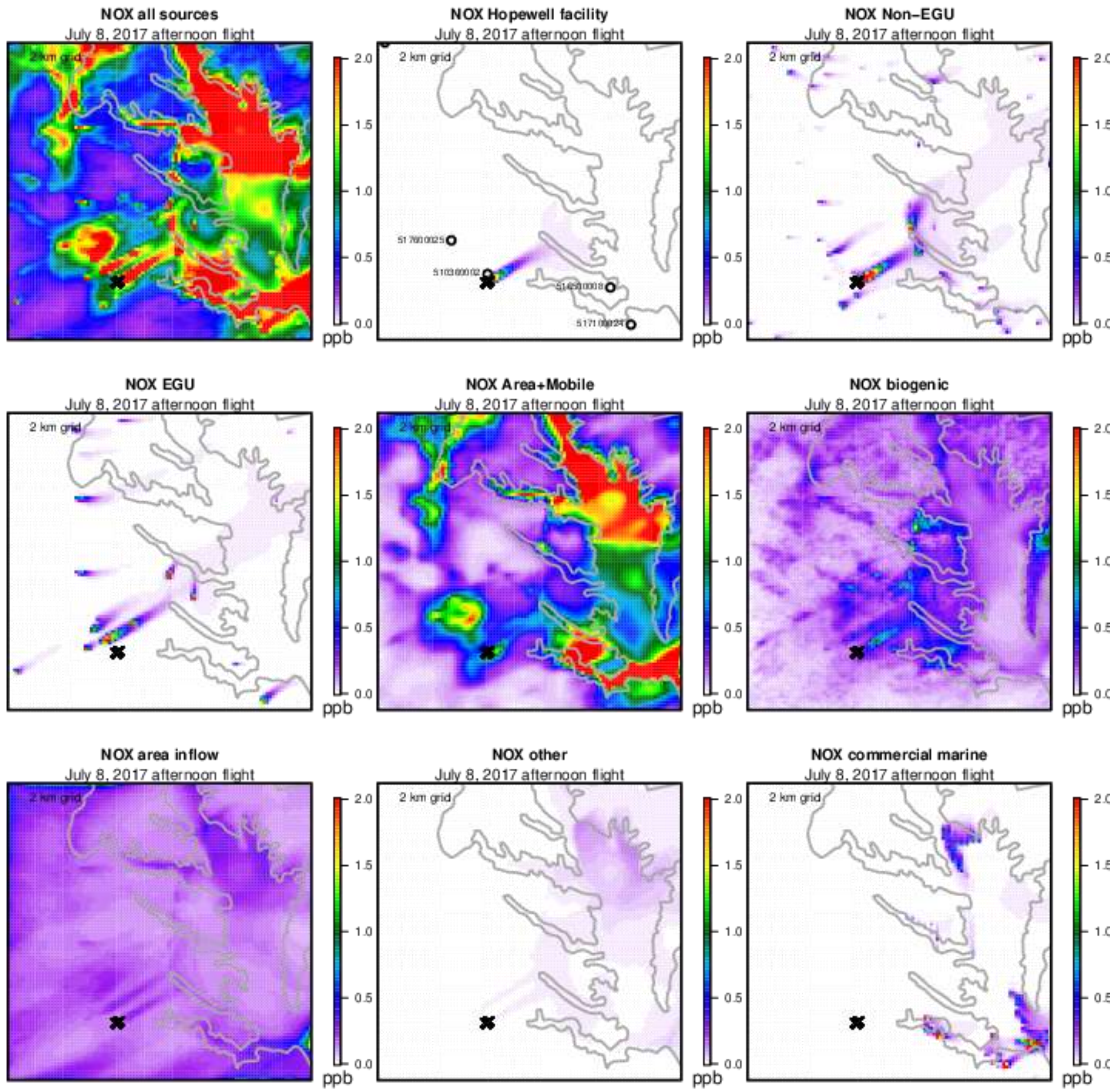

Figure S11. CMAQ 2 km (top panels) ISAM model OPTION 4 predicted surface level NO_X at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

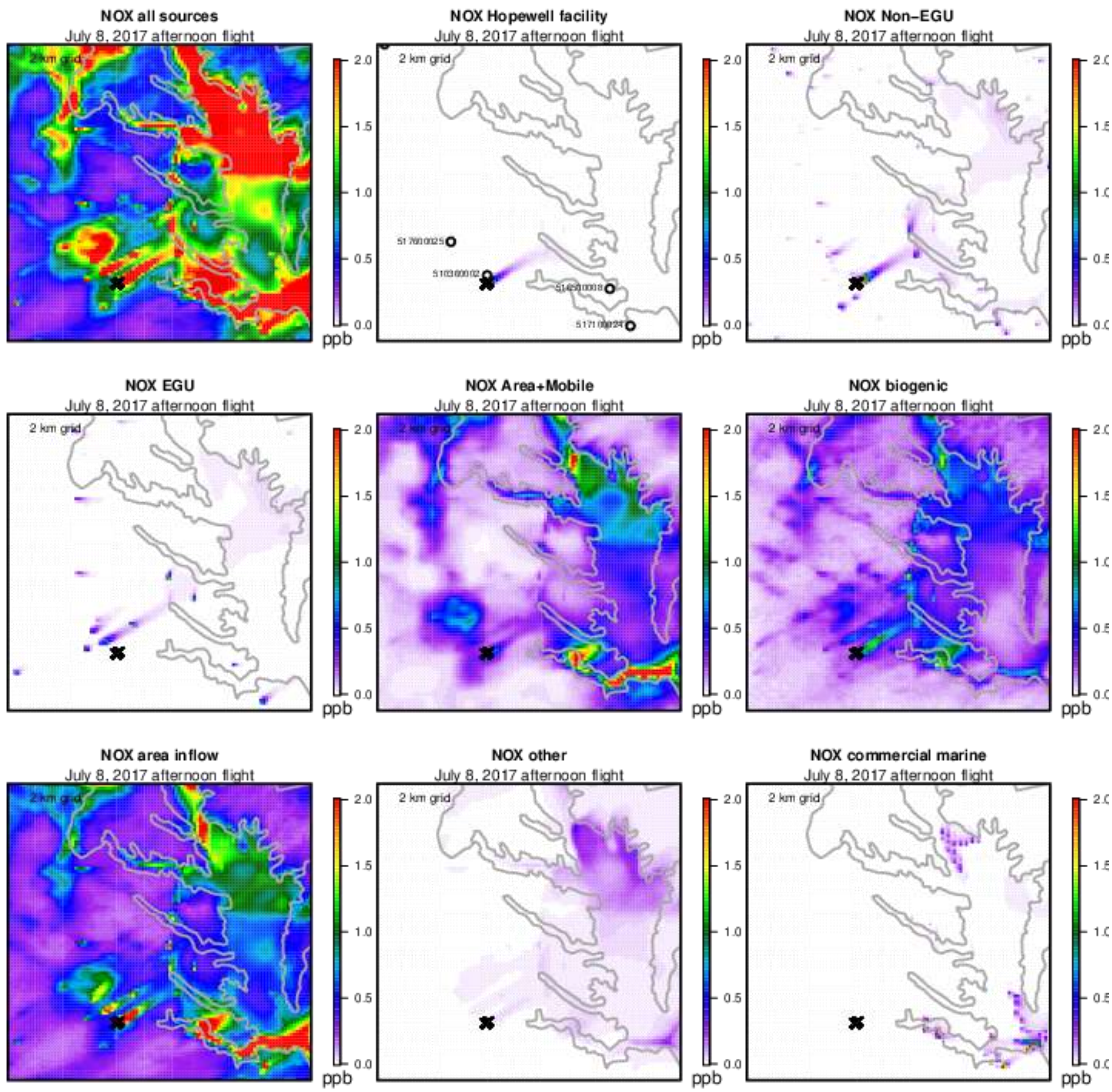

Figure S12. CMAQ 2 km (top panels) ISAM model OPTION 5 predicted surface level NO_X at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

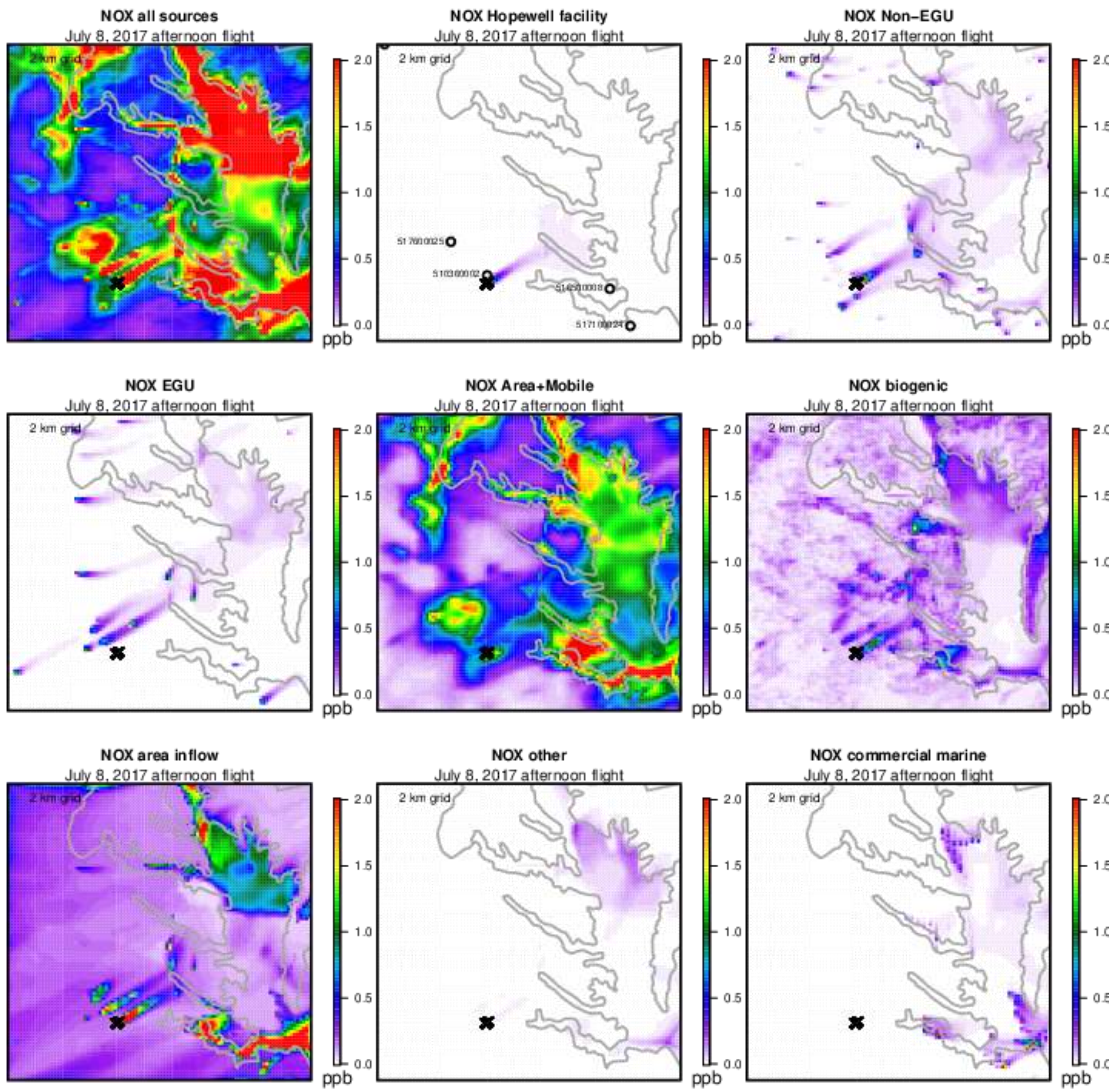

Figure S13. CMAQ 2 km (top panels) DDM model predicted surface level NO_X at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

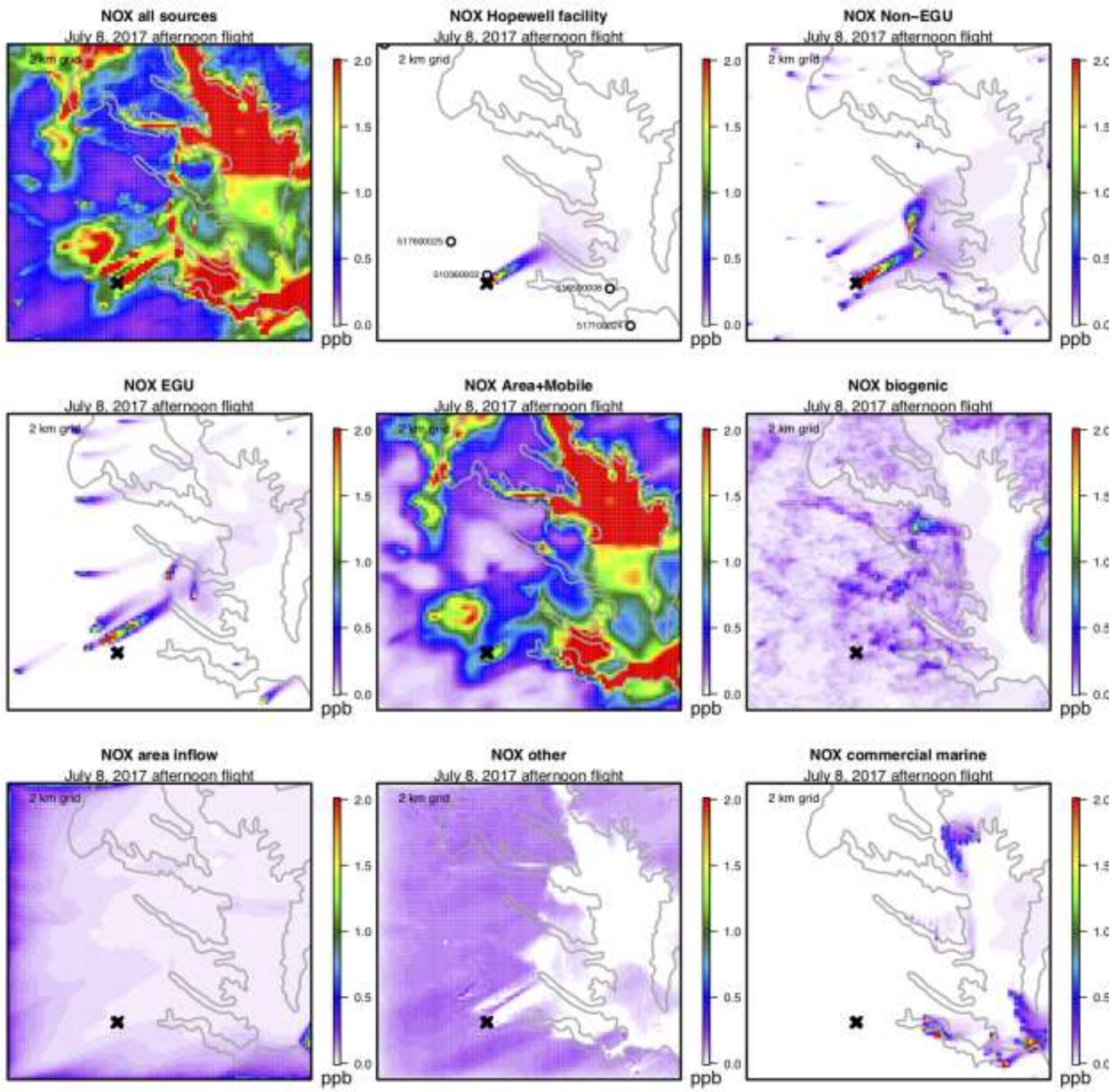

Figure S14. CMAQ 2 km (top panels) ISAM model OPTION 1 predicted surface level O_3 at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

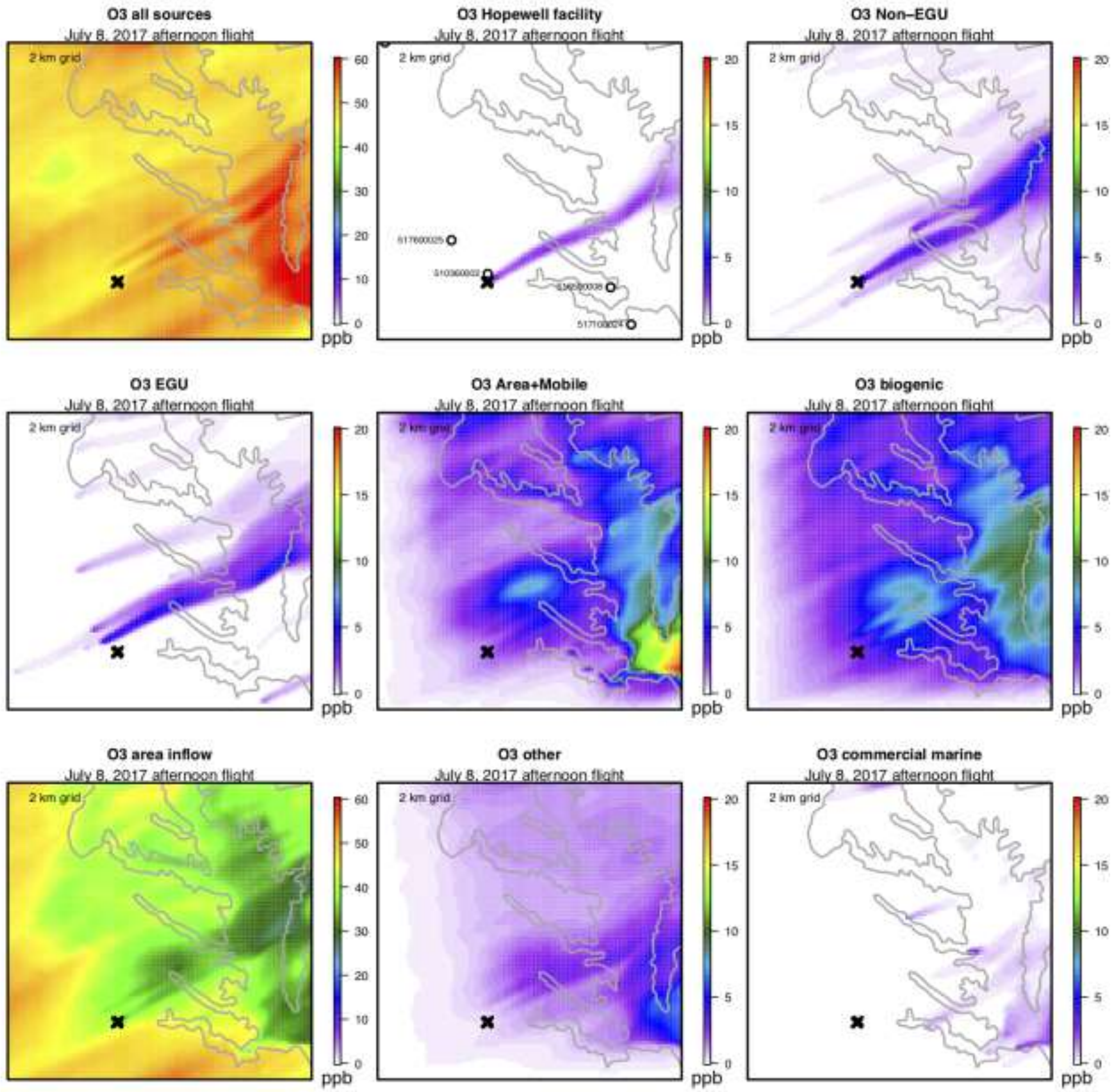

Figure S15. CMAQ 2 km (top panels) ISAM model OPTION 2 predicted surface level O_3 at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

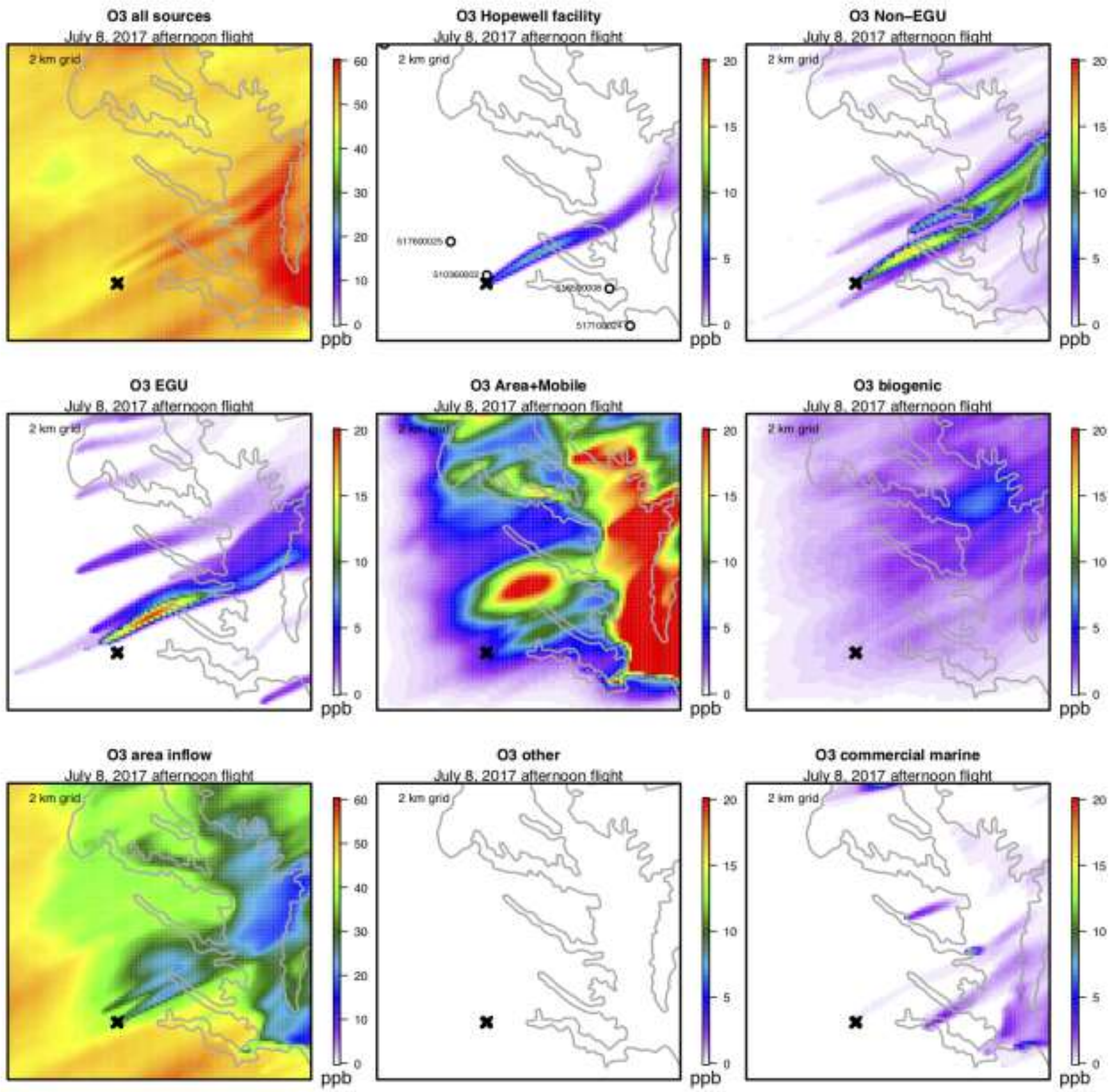

Figure S16. CMAQ 2 km (top panels) ISAM model OPTION 3 predicted surface level O_3 at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

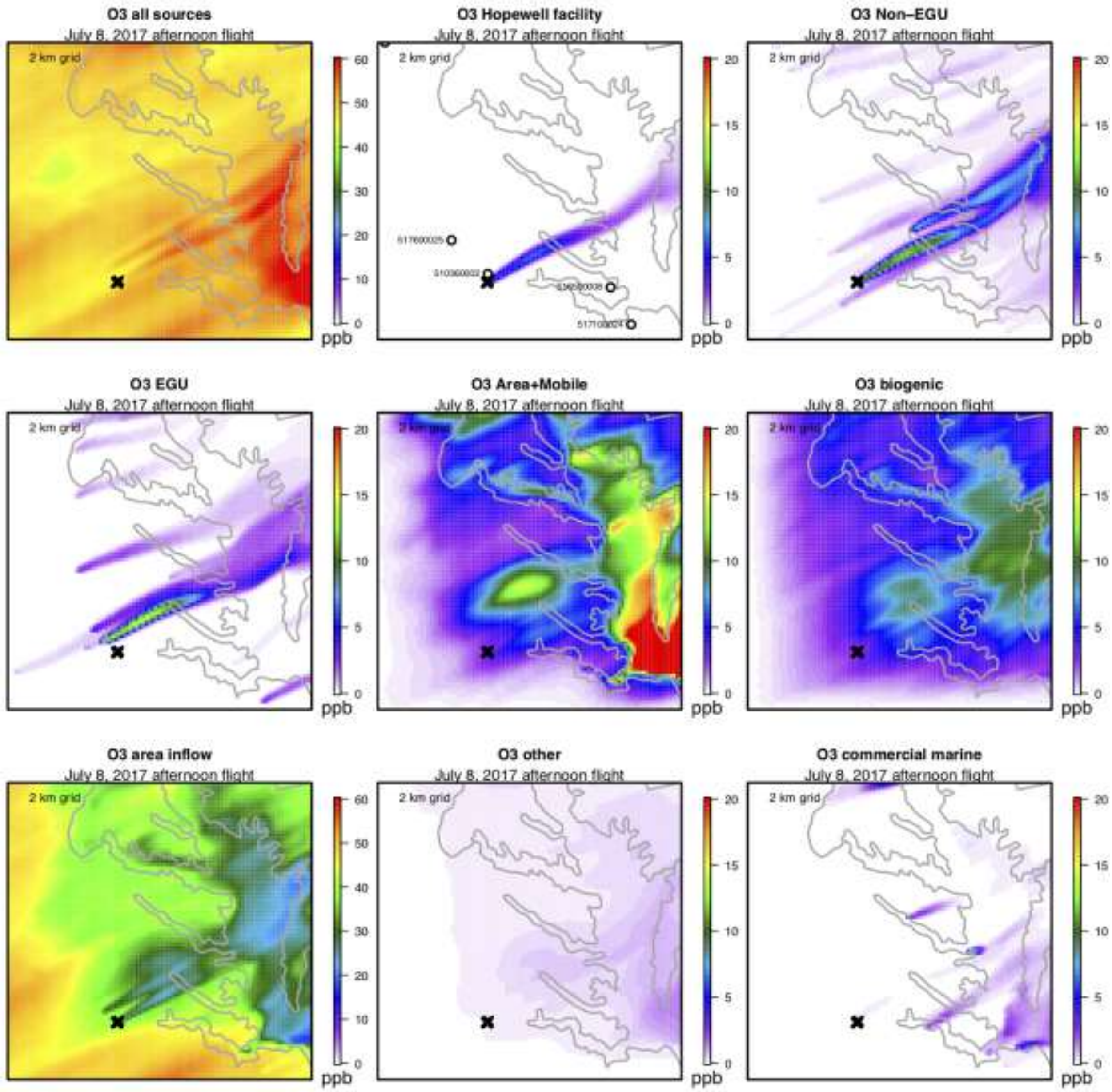

Figure S17. CMAQ 2 km (top panels) ISAM model OPTION 4 predicted surface level O_3 at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

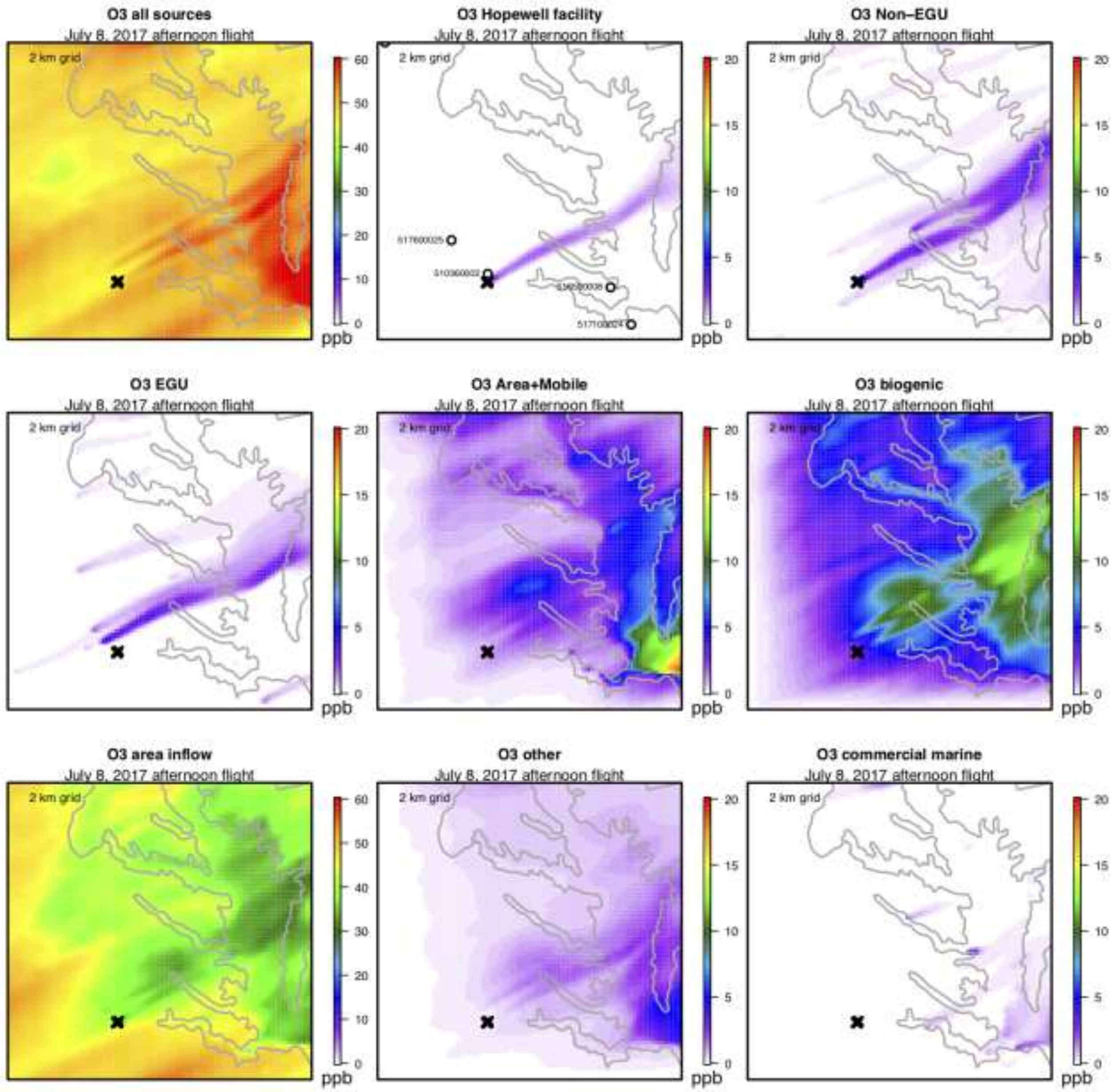

Figure S18. CMAQ 2 km (top panels) ISAM model OPTION 5 predicted surface level O_3 at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area.

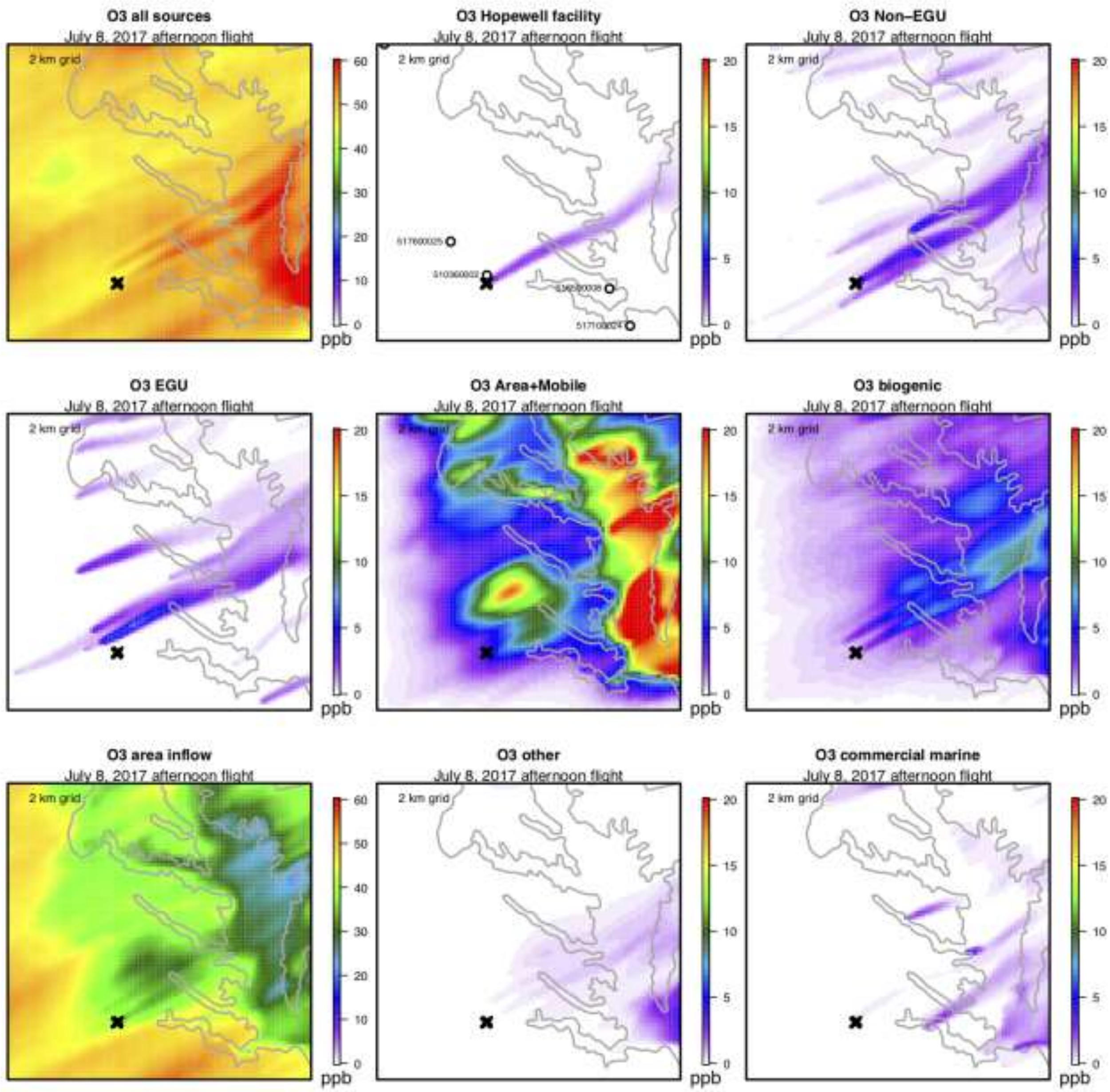

Figure S19. CMAQ 2 km (top panels) DDM model predicted surface level O_3 at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area. Sensitivities based on NO_X emissions only.

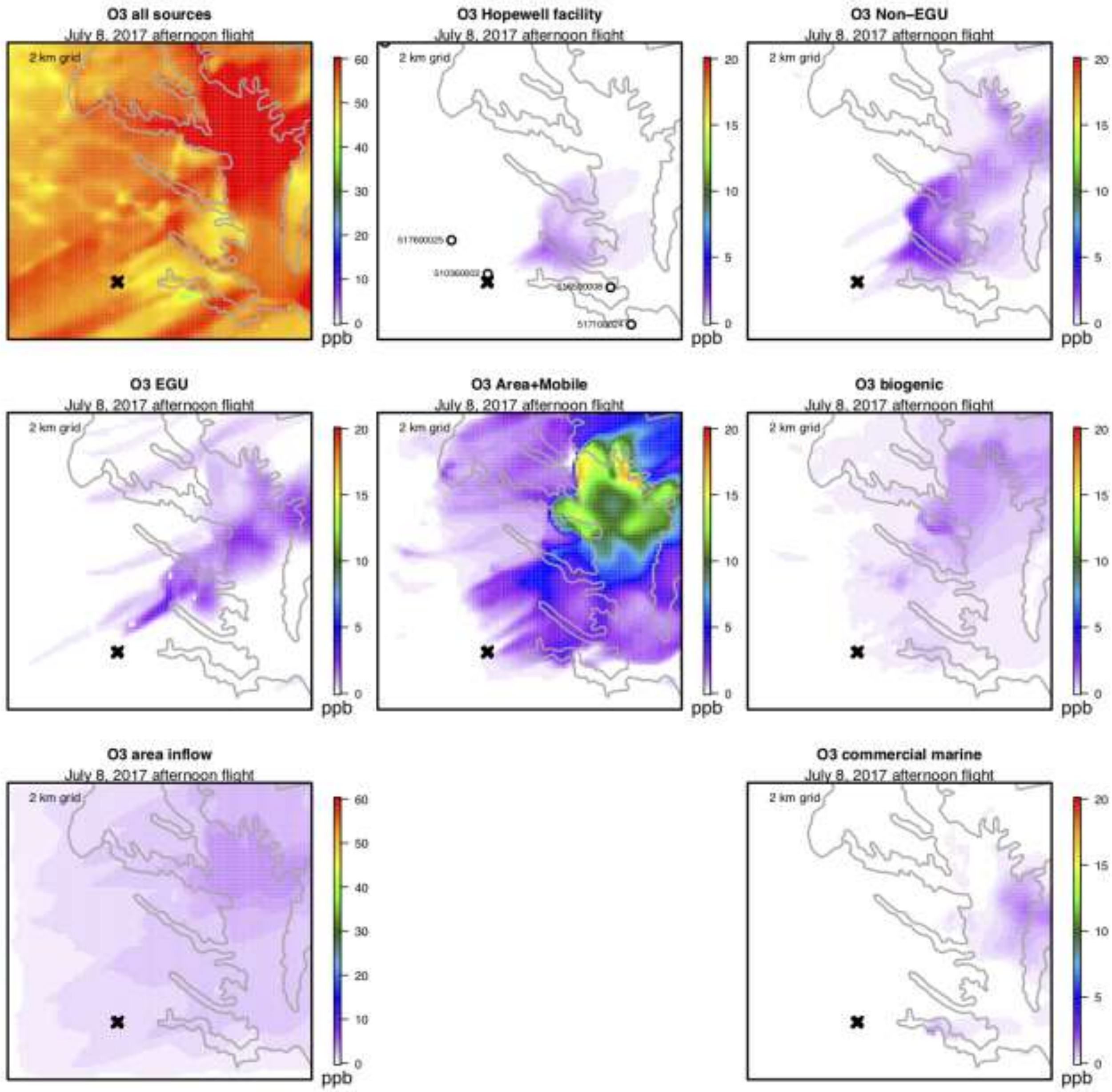

Figure S20. CMAQ 2 km (top panels) DDM model predicted surface level O_3 at the time of the July 8, 2017 afternoon aircraft measurements. Open circles show the location of routine surface monitor sites in the area. Sensitivities based on NO_X and VOC emissions. Boundary inflow also includes influence from O_3 in addition to NO_X and VOC species.