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South Asia anthropogenic ammonia emission inversion through assimilating IASI observations

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1 Minimization of the Cost Function in 4DEnVar

The minimization of the cost function follows the 4DEnVar processes. An ensemble of emission inventory is generated randomly using the prior emission vector f_h and the assumed emission error covariance $\mathbf{B}$:

$$[\boldsymbol{f}_1, \ldots, \boldsymbol{f}_N] \tag{S1}$$

An ensemble of GEOS-Chem model simulations then forward with the ensemble emission inventories in parallel:

$$[\mathcal{M}(\boldsymbol{f}_1), \ldots, \mathcal{M}(\boldsymbol{f}_N)] \tag{S2}$$

Denote the emission ensemble perturbation matrix by:

$$\mathbf{F}' = \frac{1}{\sqrt{N-1}} \left[\boldsymbol{f}_1 - \overline{\boldsymbol{f}}, \ldots, \boldsymbol{f}_N - \overline{\boldsymbol{f}}\right] \tag{S3}$$

and mean of ensemble simulation by:

$$\overline{\mathcal{M}(\boldsymbol{f})} = \frac{1}{N} \sum_{i=1}^{N} \mathcal{M}(\boldsymbol{f}_i) \tag{S4}$$

where f is the mean of the ensemble emission inventories. In the 4DEnVar assimilation algorithm, the optimal emission f is defined as weighted sum of the columns of the perturbation matrix $\mathbf{F}'$ using weights from a control variable vector $\boldsymbol{w}$:

$$\boldsymbol{f} = \overline{\boldsymbol{f}} + \mathbf{F}'\boldsymbol{w} \tag{S5}$$

The cost function could then be reformulated as:

$$\mathcal{J}(\boldsymbol{w}) = \frac{1}{2}\boldsymbol{w}^{\mathrm{T}}\boldsymbol{w} + \frac{1}{2}\left\{\mathbf{H}\mathbf{M}'\boldsymbol{w} + \mathbf{H}\overline{\mathcal{M}(\boldsymbol{f})} - \boldsymbol{y}\right\}^{\mathrm{T}} \mathbf{O}^{-1} \left\{\mathbf{H}\mathbf{M}'\boldsymbol{w} + \mathbf{H}\overline{\mathcal{M}(\boldsymbol{f})} - \boldsymbol{y}\right\} \tag{S6}$$

here $\mathbf{M}$ is the linearization of the GEOS-Chem ammonia simulating model required for cost function minimization, and is approximated by:

$$\mathbf{M}\mathbf{F}' \approx \frac{1}{\sqrt{N}} \left[\mathcal{M}(f_1) - \overline{\mathcal{M}(f)}, \ldots, \mathcal{M}(f_N) - \overline{\mathcal{M}(f)}\right] \tag{S7}$$

with the uncertainty in emission transferred into the observations space, the minimum of the cost function in Eq.(S6) could then be directly calculated, and the posterior emission f subsequently be updated.

$$m_z = \frac{M_z^m - B_z}{M^m - B} \tag{S8}$$

here M_z^m represents the modeled concentration of NH_3 at altitude z. B_z is the background concentration of NH_3 at the same altitude. M_z represents the total modeled concentration of NH_3 in the atmosphere. B is the total background concentration.

$$A_z^a = \frac{1}{N} \frac{\hat{X}^a - B}{\hat{X}^{|z} - B} \tag{S9}$$

here X_z^a represents the a priori (or assumed) concentration of NH_3 at altitude z. B_z is again the background concentration at that altitude. X^a is the total a priori concentration. N is a normalization factor, ensuring the matrix A_z^a sums correctly to account for all altitudes.

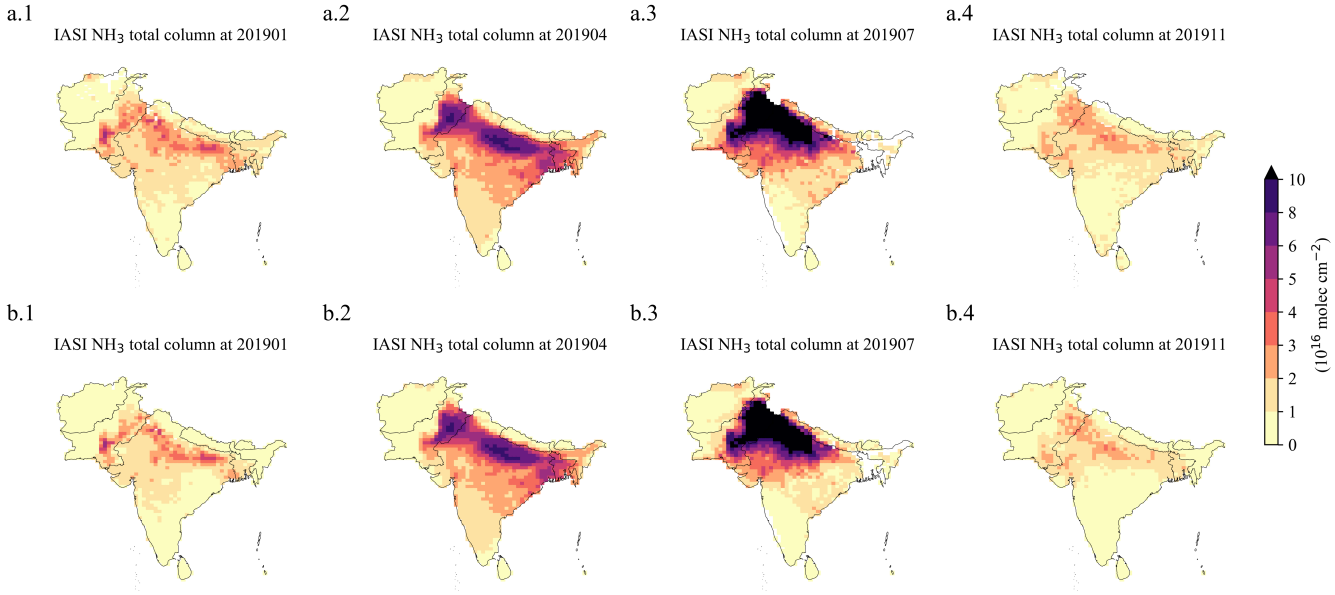

Figure S1. The distribution of IASI NH_3 total column data in 2019. Panels (a.1)–(a.4) display the data after excluding negative values, while panels (b.1)–(b.4) display the data with negative values retained, corresponding to January, April, July, and November, respectively

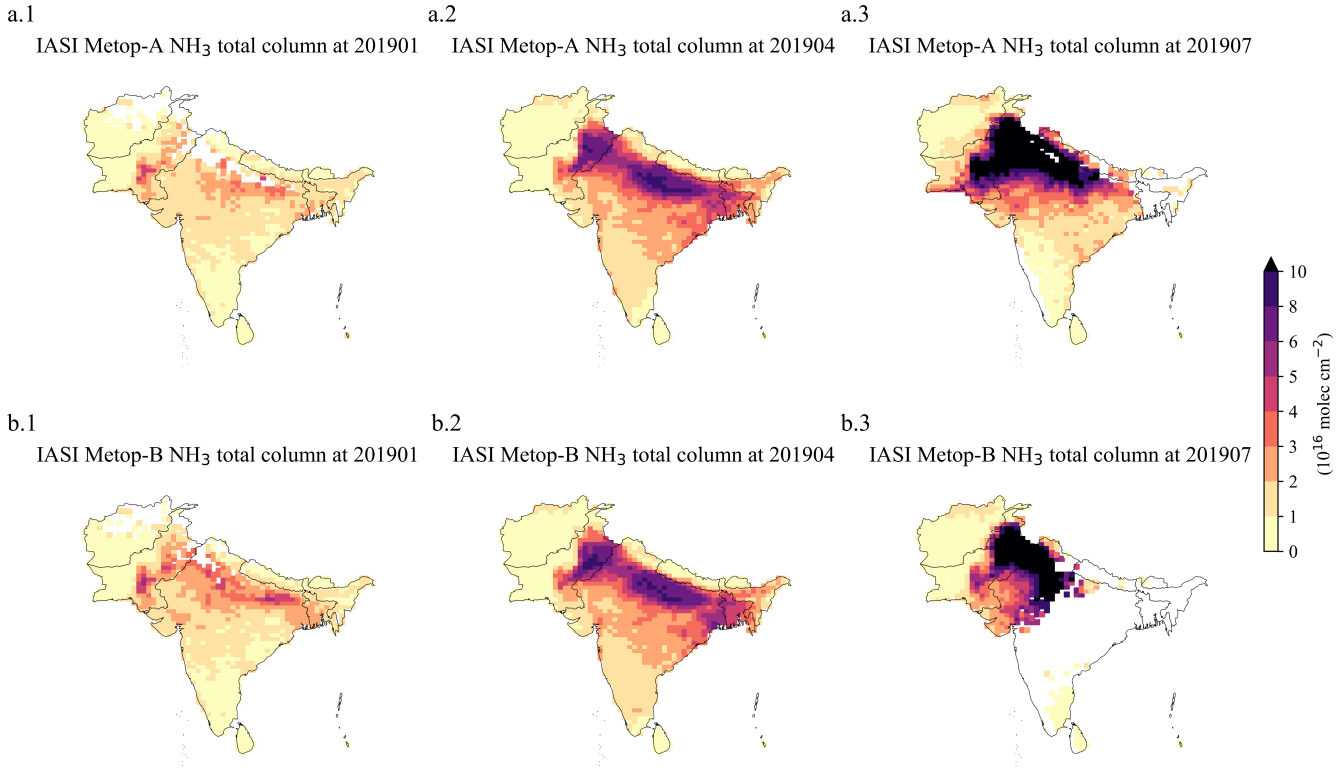

Figure S2. The distribution of IASI Metop-A (a) and Metop-B (b) NH_3 total column in 2019 January (a.1-b.1), April (a.2-b.2) and July (a.3-b.3).

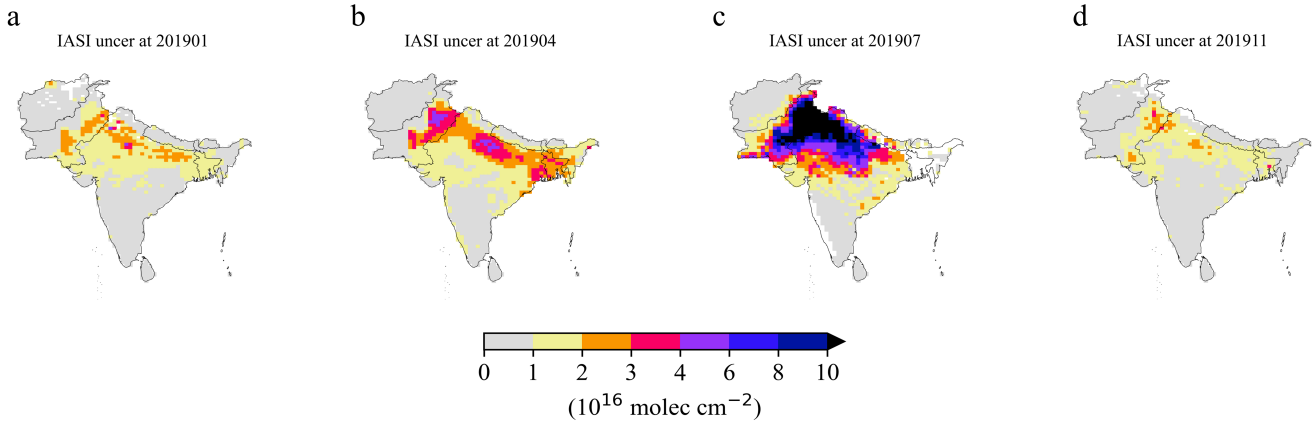

Figure S3. The distribution of IASI instruments' uncertainty in 2019 January (a), April (b), July (c) and November (d).

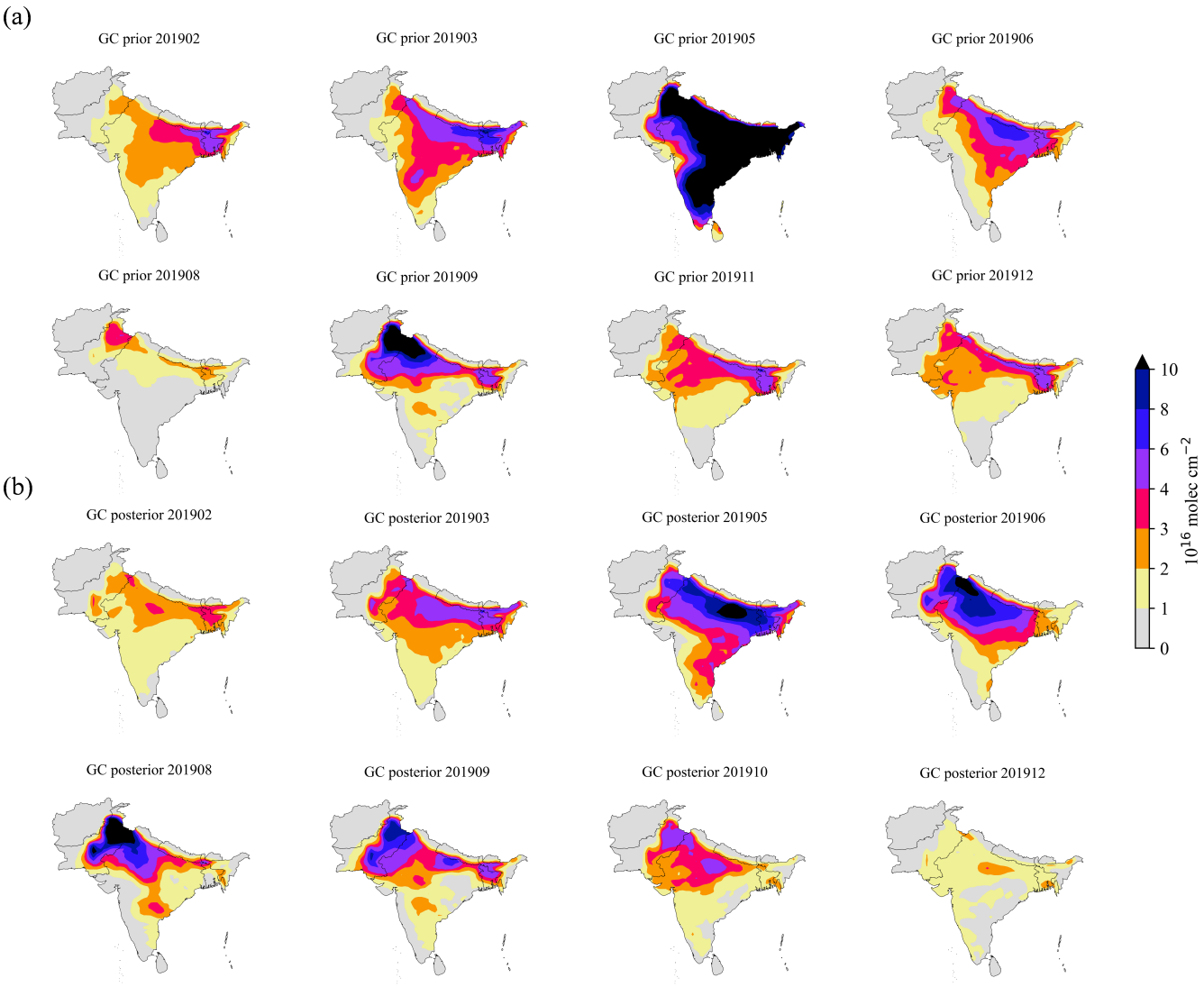

Figure S4. The distribution of the prior (a) and the posterior (b) ammonia total column for the remain months in 2019.

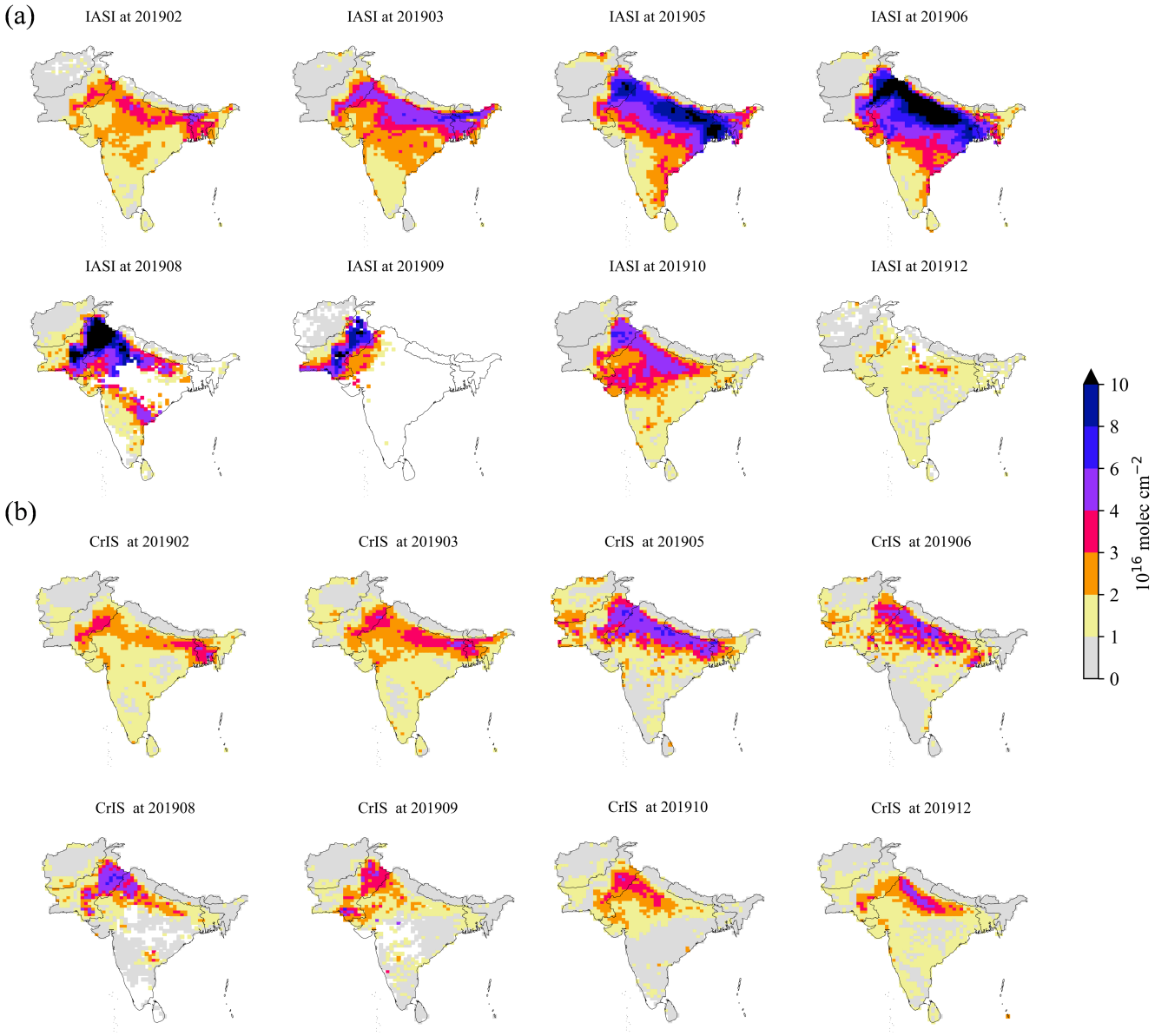

Figure S5. The distribution of the IASI-observed (a) and the CrIS-observed (b) ammonia total column for the remain months in 2019.

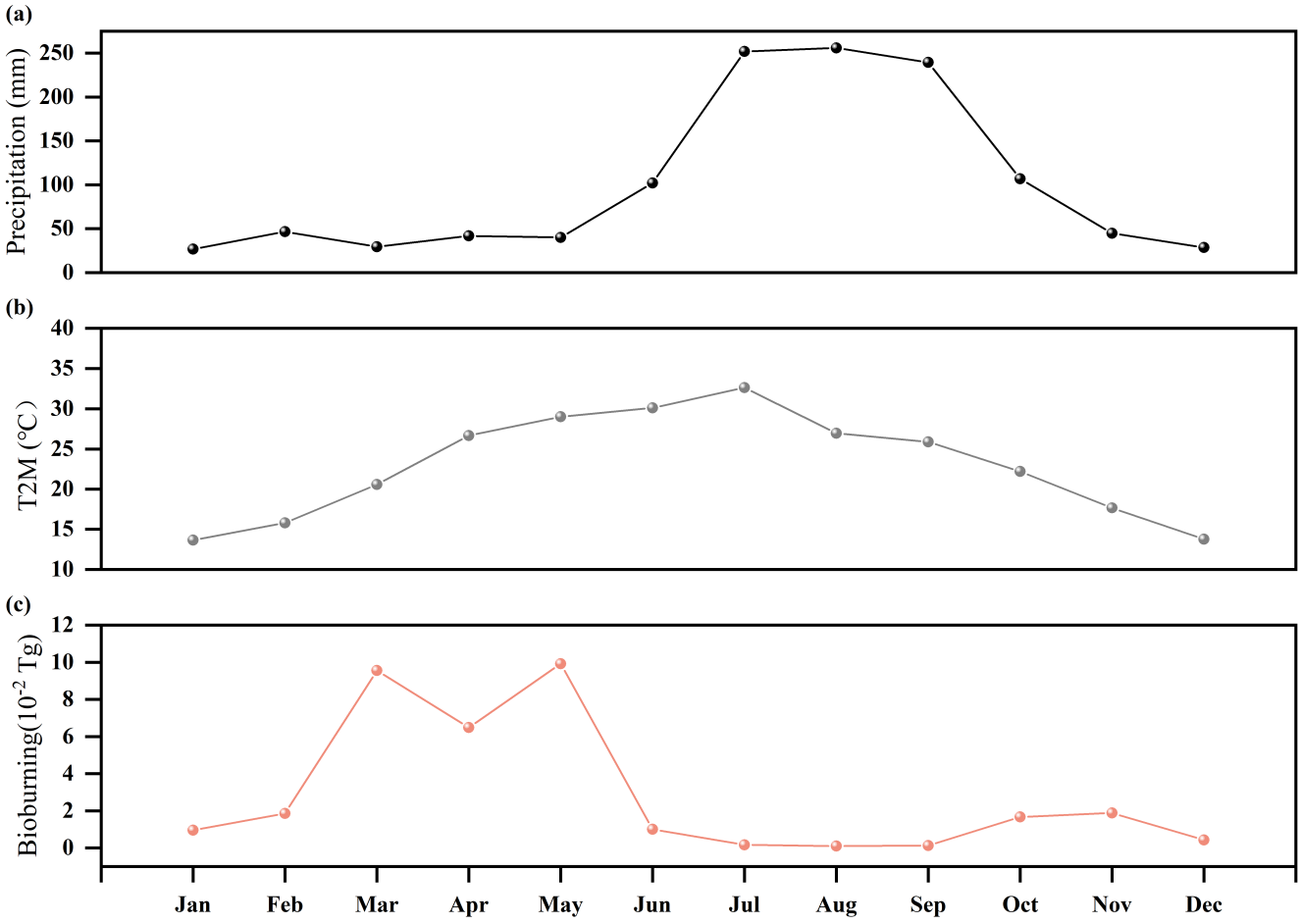

Figure S6. Monthly precipitation (a), temperature (b) from MERRA2 and biomass buring emission (c) from GFED4 in 2019.

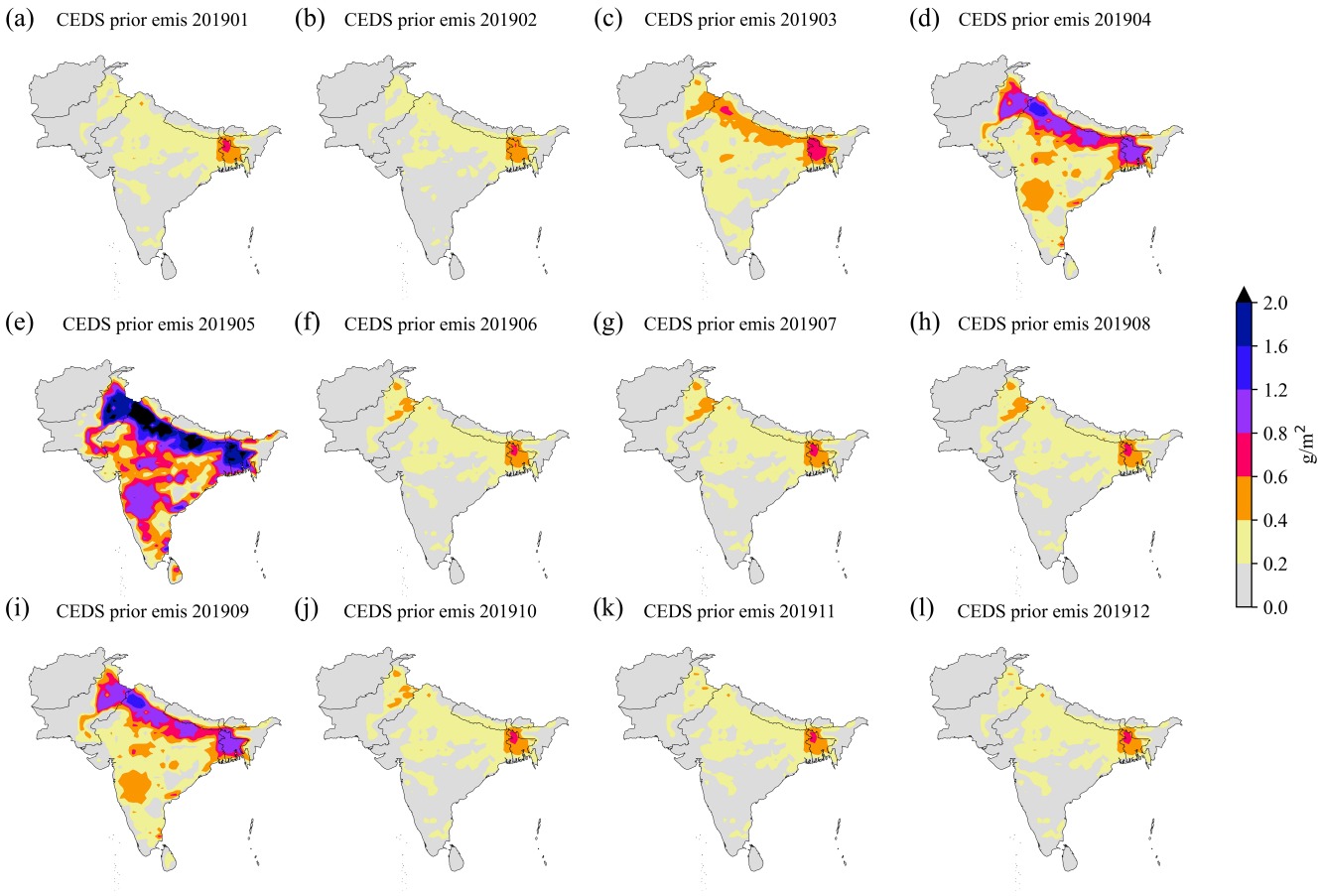

Figure S7. (a)-(l) represent the distribution of the prior inventory for each month from January to December in 2019.

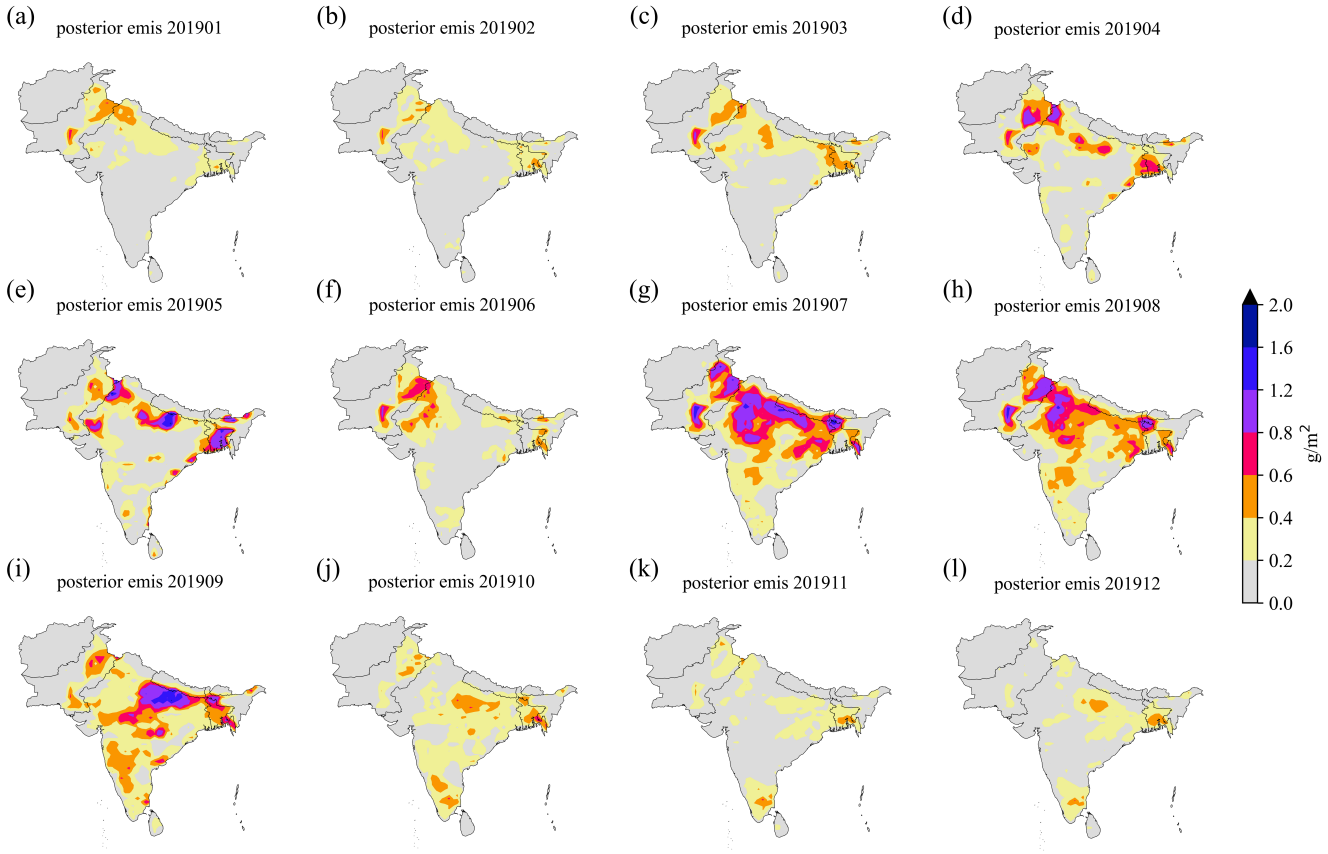

Figure S8. (a)-(l) represent the distribution of the posterior inventory for each month from January to December in 2019.

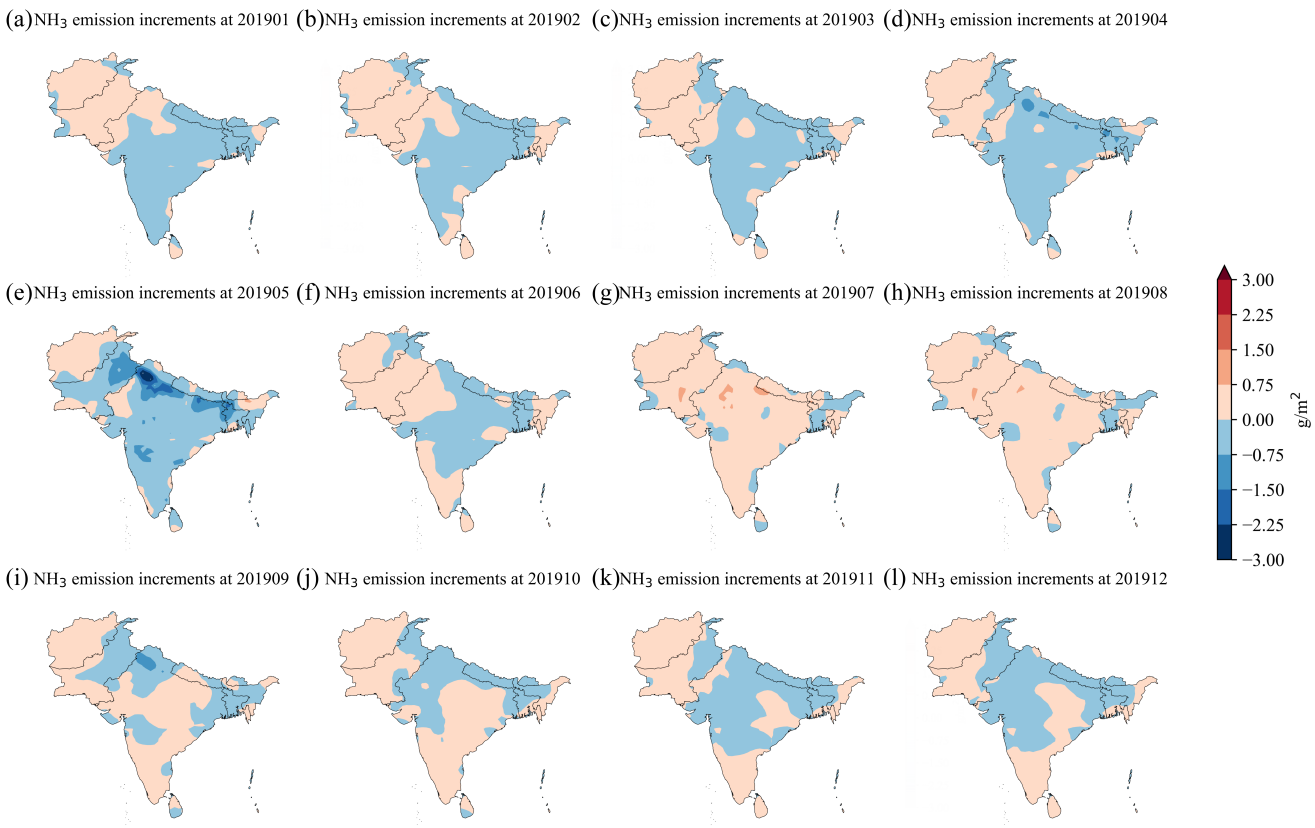

Figure S9. (a)-(l) represent the distribution of increments obtained by subtracting the prior inventory from the posterior inventory for each month from January to December in 2019.

Station	lon	lat	StationName	City	State
AP001	80.5181667	16.5150833	Secretariat, Amaravati - APPCB	Amaravati	Andhra Pradesh
AP005	83.3	17.72	GVM Corporation, Visakhapatnam - APPCB	Visakhapatnam	Andhra Pradesh
DL001	77.152491	28.815691	Alipur, Delhi - DPCC	Delhi	Delhi
DL002	77.749675	28.725645	Anand Vihar, Delhi - DPCC	Delhi	Delhi
DL019	77.2005	28.6341	Mandir Marg, Delhi - DPCC	Delhi	Delhi
DL020	77.030469	28.68241	Mundka, Delhi - DPCC	Delhi	Delhi
DL024	80.3229863	26.4703136	Nehru Nagar, Delhi - DPCC	Delhi	Delhi
HR012	77.0667	28.4227	Sector-51, Gurugram - HSPCB	Gurugram	Haryana
KA011	77.622813	12.917348	Silk Board, Bengaluru - KSPCB	Bengaluru	Karnataka
MH008	72.82	18.91	Gole Bazar, Katni - MPPCB	Katni	Madhya Pradesh
PB001	74.876512	31.62	Golden Temple, Amritsar - PPCB	Amritsar	Punjab
RJ004	75.836858	26.902909	Adarsh Nagar, Jaipur - RSPCB	Jaipur	Rajasthan
RJ005	75.7994901	26.9164092	Police Commissionerate, Jaipur - RSPCB	Jaipur	Rajasthan
RJ006	75.730943	26.9502929	Shastri Nagar, Jaipur - RSPCB	Jaipur	Rajasthan
TN001	80.1076538	12.9099161	Alandur Bus Depot, Chennai - CPCB	Chennai	Tamil Nadu
TG006	78.451437	17.349694	Zoo Park, Hyderabad - TSPCB	Hyderabad	Telangana
UP012	80.9302753	26.8821003	Central School, Lucknow - CPCB	Lucknow	Uttar Pradesh
UP013	81.005119	26.86812	Gomti Nagar, Lucknow - UPPCB	Lucknow	Uttar Pradesh
WB007	88.3638022	22.5367507	Ballygunge, Kolkata - WBPCB	Kolkata	West Bengal
WB008	88.41002457	22.58157048	Bidhannagar, Kolkata - WBPCB	Kolkata	West Bengal
AS001	91.78063	26.181742	Railway Colony, Guwahati - APCB	Guwahati	Assam
MH012	72.8204	19.3832	Vasai West, Mumbai - MPCB	Mumbai	Maharashtra
WB011	88.380669	22.627847	Rabindra Bharati University, Kolkata - WBPCB	Kolkata	West Bengal
ML001	91.8985	25.5586	Lumpyngngad, Shillong - Meghalaya PCB	Shillong	Meghalaya
BR005	85.043586	25.586562	DRM Office Danapur, Patna - BSPCB	Patna	Bihar
BR006	85.227158	25.592539	Govt. High School Shikarpur, Patna - BSPCB	Patna	Bihar

Table S1. Stations with both $PM_{2.5}$ data and NH_3 data

Station	lon	lat	StationName	City	State
AP002	81.7363176	16.9872867	Anand Kala Kshetram, Rajamahendravaram - APPCB	Rajamahendravaram	Andhra Pradesh
BR001	84.9994	24.7955	Collectorate, Gaya - BSPCB	Gaya	Bihar
BR003	85.2459	25.697189	Industrial Area, Hajipur - BSPCB	Hajipur	Bihar
HR001	76.778328	30.379589	Patti Mehar, Ambala - HSPCB	Ambala	Haryana
HR002	76.9254	28.6701	Arya Nagar, Bahadurgarh - HSPCB	Bahadurgarh	Haryana
HR003	77.319699	28.3419248	Nathu Colony, Ballabgarh - HSPCB	Ballabgarh	Haryana
HR004	76.141105	28.806223	H.B. Colony, Bhiwani - HSPCB	Bhiwani	Haryana
HR005	76.7997	28.2068	Municipal Corporation Office, Dharuhera - HSPCB	Dharuhera	Haryana
HR010	75.467934	29.503664	Huda Sector, Fatehabad - HSPCB	Fatehabad	Haryana
HR015	75.744941	29.14056	Urban Estate-II, Hisar - HSPCB	Hisar	Haryana
HR016	76.337619	29.307814	Police Lines, Jind - HSPCB	Jind	Haryana
HR017	76.4155	29.8006	Rishi Nagar, Kaithal - HSPCB	Kaithal	Haryana
HR018	77.0027	29.6953	Sector-12, Karnal - HSPCB	Karnal	Haryana
HR019	76.875879	29.966942	Sector-7, Kurukshetra - HSPCB	Kurukshetra	Haryana
HR020	76.9938	27.9002	General Hospital, Mandikhera - HSPCB	Mandikhera	Haryana
HR021	76.93609	28.360699	Sector-2 IMT, Manesar - HSPCB	Manesar	Haryana
HR022	75.730943	26.9502929	Shastri Nagar, Narnaul - HSPCB	Narnaul	Haryana
KA001	75.659694	16.172806	Vidayagiri, Bagalkot - KSPCB	Bagalkot	Karnataka
KA012	76.55521	11.55358	Urban, Chamarajanagar - KSPCB	Chamarajanagar	Karnataka
KA013	77.731418	13.428828	Chikkaballapur Rural, Chikkaballapur - KSPCB	Chikkaballapur	Karnataka
KA014	75.797056	13.328028	Kalyana Nagara, Chikkamagaluru - KSPCB	Chikkamagaluru	Karnataka
KL001	76.302765	10.073232	Udyogamandal, Eloor - Kerala PCB	Eloor	Kerala
MP002	79.446246	23.81748678	Shrivastav Colony, Damoh - MPPCB	Damoh	Madhya Pradesh
MP003	76.064118	22.9682591	Bhopal Chauraha, Dewas - MPPCB	Dewas	Madhya Pradesh
MP004	78.193251	26.203442	City Center, Gwalior - MPPCB	Gwalior	Madhya Pradesh
MP006	75.5213	22.431	Chhoti Gwaltoli, Indore - MPPCB	Indore	Madhya Pradesh
MP007	79.932247	23.168606	Marhatal, Jabalpur - MPPCB	Jabalpur	Madhya Pradesh
MP008	80.23284	23.50016	Gole Bazar, Katni - MPPCB	Katni	Madhya Pradesh
MH002	77.6345232	19.645324	Chandrapur, Chandrapur - MPCB	Chandrapur	Maharashtra
MH004	73.142019	19.25292	Khadakpada, Kalyan - MPCB	Kalyan	Maharashtra
PB002	74.907758	30.233011	Hardev Nagar, Bathinda - PPCB	Bathinda	Punjab
PB003	75.578914	31.321907	Civil Line, Jalandhar - PPCB	Jalandhar	Punjab
PB004	76.209694	30.736056	Kalal Majra, Khanna - PPCB	Khanna	Punjab
PB005	75.8086	30.9028	Punjab Agricultural University, Ludhiana - PPCB	Ludhiana	Punjab
PB006	76.331442	30.649961	RIMT University, Mandi Gobindgarh - PPCB	Gobindgarh	Punjab
PB007	76.366642	30.349388	Model Town, Patiala - PPCB	Patiala	Punjab
PB008	76.5623046	31.0325454	Ratanpura, Rupnagar - Ambuja Cements	Rupnagar	Punjab
RJ001	76.611536	27.554793	Moti Doongri, Alwar - RSPCB	Alwar	Rajasthan
RJ002	74.646594	26.470859	Civil Lines, Ajmer - RSPCB	Ajmer	Rajasthan
RJ003	76.862296	28.194909	RIICO Ind. Area III, Bhiwadi - RSPCB	Bhiwandi	Rajasthan
RJ007	84.9994	24.7955	Collectorate, Jodhpur - RSPCB	Jodhpur	Rajasthan
RJ008	75.821256	25.14389	Shrinath Puram, Kota - RSPCB	Kota	Rajasthan
RJ009	73.340227	25.771061	Indira Colony Vistar, Pali - RSPCB	Pali	Rajasthan
RJ010	73.6321397	24.5886166	Ashok Nagar, Udaipur - RSPCB	Udaipur	Rajasthan
UP003	77.849831	28.406963	Yamunapuram, Bulandshahr - UPPCB	Bulandshahr	Uttar Pradesh
UP006	77.453839	28.685382	Sanjay Nagar, Ghaziabad - UPPCB	Ghaziabad	Uttar Pradesh
UP008	77.482	28.47272	Knowledge Park - III, Greater Noida - UPPCB	Greater Noida	Uttar Pradesh
UP010	77.749675	28.725645	Anand Vihar, Hapur - UPPCB	Hapur	Uttar Pradesh
UP011	80.3229863	26.4703136	Nehru Nagar, Kanpur - UPPCB	Kanpur	Uttar Pradesh
WB002	87.2892225	23.5404352	Sidhu Kanhu Indoor Stadium, Durgapur - WBPCB	Durgapur	West Bengal
WB003	88.109737	22.06047	Haldia, Haldia - WBPCB	Haldia	West Bengal
GJ002	73.010555	21.613267	GIDC, Ankleshwar - GPCB	Ankleshwar	Gujarat
GJ004	73.010555	21.613267	GIDC, Nandesari - Nandesari Ind. Association	Nandesari	Gujarat
GJ005	72.918013	20.362421	Phase-1 GIDC, Vapi - GPCB	Vapi	Gujarat
HR023	77.3320667	28.1485564	Shyam Nagar, Palwal - HSPCB	Palwal	Haryana
MH015	79.0517531	21.152875	Opp GPO Civil Lines, Nagpur - MPCB	Nagpur	Maharashtra
MH016	73.7762427	20.0073285	Gangapur Road, Nashik - MPCB	Nashik	Maharashtra
MH021	75.9063906	17.6599188	Solapur, Solapur - MPCB	Solapur	Maharashtra
UP018	77.7622941	28.9535882	Jai Bhim Nagar, Meerut - UPPCB	Meerut	Uttar Pradesh
UP019	77.709723	29.06351	Pallavpuram Phase 2, Meerut - UPPCB	Meerut	Uttar Pradesh
UP021	77.7194031	29.4723508	New Mandi, Muzaffarnagar - UPPCB	Muzzaffarnagar	Uttar Pradesh
UP022	77.3231257	28.5447608	Sector - 125, Noida - UPPCB	Noida	Uttar Pradesh
KA015	75.140726	15.351773	Deshpande Nagar, Hubballi - KSPCB	Hubballi	Karnataka
WB014	88.412668	26.6883049	Ward-32 Bapupara, Siliguri - WBPCB	Siliguri	West Bengal
KA017	76.37376	12.21041	Hebbal 1st Stage, Mysuru - KSPCB	Mysuru	Karnataka
KA018	77.298051	12.733409	Vijay Nagar, Ramanagara - KSPCB	Ramanagara	Karnataka
MP010	77.511428	23.10844	Sector-D Industrial Area, Mandideep - MPPCB	Mandideep	Madhya Pradesh
MP011	75.675238	22.624758	Sector-2 Industrial Area, Pithampur - MPPCB	Pithampur	Madhya Pradesh
MP012	75.045981	23.331731	Shasthri Nagar, Ratlam - IPCA Lab	Ratlam	Madhya Pradesh
UP025	77.393848	28.56923	Sector-116, Noida - UPPCB	Noida	Uttar Pradesh
UP026	82.9083074	25.3505986	Ardhali Bazar, Varanasi - UPPCB	Varanasi	Uttar Pradesh
KA016	76.822628	17.321993	Lal Bahadur Shastri Nagar, Kalaburagi - KSPCB	Kalaburagi	Karnataka

Table S2. Stations with $PM_{2.5}$ data but without NH_3 data

Station	lon	lat	StationName	City	State
BR008	85.147382	25.619651	Muradpur, Patna - BSPCB	Patna	Bihar
KL007	76.8865	8.5637	Kariavattom, Thiruvananthapuram - Kerala PCB	Thiruvananthapuram	Kerala
MZ001	92.7192841	23.7176342	Sikulpuikawn, Aizawl - Mizoram PCB	Aizawl	Mizoram
OD001	83.8396977	21.8004996	GM Office, Brajrajnagar - OSPCB	Brajrajnagar	Odisha
OD002	85.1707021	20.9360711	Talcher Coalfields, Talcher - OSPCB	Talcher	Odisha

Table S3. Stations with NH_3 data but without $PM_{2.5}$ data