equations

# emission

- $E = M/\tau$
  - $E$: emission fluxes, assumes stationarity and constant first-order loss terms
  - $M$: the total mass contained within the assumed box
  - τ: The effective lifetime or residence time of NH3 within a given box
- $\tau_{\mathrm{m}od} = \frac{M_{mod}}{E_{mod}}$
- $E_{obs} = \frac{M_{\mathrm{obs}}}{\tau_{\mathrm{m}od}} = M_{\mathrm{obs}} * \frac{E_{mod}}{M_{mod}} = E_{mod} * \frac{C_{\mathrm{obs}}}{C_{mod}}$

# Oversampling/lifetime

- $v(x, y) = \frac{\sum_{i=1}^{n} w_i v_i}{\sum_{i=1}^{n} w_i}$
  - $v(x, y)$: the interpolated value at point ($x$, $y$)
  - $w_i$: the relative weights
  - $v_i$: the observation values
- $w_i = (\frac{r_w - d_i}{r_w d_i})^2$
  - $r_w$ : the radius of influence of the point ($x_i$, $y_i$)
  - $d_i$: the distance between point ($x$, $y$) and ($x_i$, $y_i$), the threshold distance is 50km
- $E_{NH3} = M_{NH3}/\tau$
- $\tau_{mod} = C_{NH3}/L_{NH3}$
  - $C_{NH3}$: the atmospheric burden of ammonia
  - $L_{NH3}$: total loss

# Modeled concentrations

- Modeled concentrations: discretize the area source region (50m spacing)
- $c_{model} = \sum_i^n \frac{Q_{ref}}{n} * K_i$
  - $Q_{ref}$: total emission, set to 1 g s-1
  - $K_i$: the dispersion kernel at the ith subregion
- $K = \frac{1}{\pi * \sigma_x * \sigma_y * \bar{u}} * e^{\frac{-y^2}{2\sigma_y^2}} * e^{\frac{-z^2}{2\sigma_z^2}}$
  - $\bar{u}$: mean wind speed——effective wind speed
  - $\sigma_x / \sigma_y$: the dispersion coefficient
- $\bar{u} = \frac{\int ucdz}{\int cdz}$
  - $u(z)$: the variation of wind speed with height z——a ratio form of logarithmic profile
- $\mathrm{u}(z) = u_{10} * \frac{\ln(\frac{z-d}{z_0} + \varphi_m(\frac{z}{L}))}{\ln(\frac{10-d}{z_0} + \varphi_m(\frac{10}{L}))}$
  - $z_0 = 0.04$m: the surface roughness
  - $d = 0.5$m: the displacement height
  - $\varphi_m(\frac{z}{L})$: stability terms
- $L = -\frac{\rho c_p T u_*^3}{kgH}$
  - $c_p$: the specific heat of air at constant pressure
  - $k$: the von Karman constant
  - $\rho$: the density of air
  - $g$: the acceleration due to gravity
- $Q_{est} = Q_{ref} \frac{\sum c_{obs}}{\sum c_{model}}$
  - $Q_{est}$: estimated emission rates

The total emissions in kg/month for animal type a

- $E_a = pop_a * \frac{1}{n} \sum_{j=1}^{n} \frac{E_{a,j}}{count_{a,j}}$
  - $j$: each observation period
  - $count_{a,j}$: the number of animals (a)
  - $pop_a$: the total population of animals (a)

NH3 VRs

- $VR = VR^0 \times f(pH) \times f(A) \times f(\mathrm{u}) \times f(T) \times f(M)$
  - $VR^0$: averaged from available VR data
  - $f(pH),\ f(A),\ f(\mathrm{u}),\ f(T),\ f(M)$: the correction coefficients that reflect the effects of pH, air temperature, and wind speed, fertilizer type, and placement on VRs, respectively
- $\mathrm{V} = VR \times N \times H$
  - $V$: NH3 volatilization
  - $N$: total N application rate
  - $H$: harvested area

# lifetime

- $\frac{1}{\tau} = \frac{1}{\tau_{trans}} + \frac{1}{\tau_{chem}} + \frac{1}{\tau_{depo}}$
  - $t_{trans}$: NH3 transport in and out
  - $t_{chem}$: NH3 chemical loss
  - $t_{depo}$: NH3 deposition (dry deposition and wet deposition)
- $\frac{dC(t)}{d\text{t}} = S(t) - \frac{C(t)}{\tau(t)}$ species mass balance equation (Croft et al., 2014)
  - $C(t)$: the NH3 concentration at time $t$
  - $S(t)$: the time-dependent source emission fluxes
  - $\tau(t)$: the removal timescale
- A quasi-equilibrium between sources and removals of ammonia (Dentener and Crutzen, 1994), $S(t) = 0 \rightarrow \frac{dC(t)}{d\text{t}} = -\frac{C(t)}{\tau(t)}$
- $\tau(t) = -\frac{C(t)}{\nabla C(t)}$
  - $\Delta C(t)$: NH3 total concentration rate of change
- $\frac{-1}{\tau_{mod}} = \frac{\nabla C_{trans}}{C} + \frac{\nabla C_{chem}}{C} + \frac{\nabla C_{drydep}}{C} + \frac{\nabla C_{wetdep}}{C} \rightarrow \tau_{mod} = \frac{C}{-(\Delta C_{trans} + \Delta C_{chem} + \Delta C_{drydep} + \Delta C_{wetdep})} = \frac{M}{-\Delta M_{trans,chem,drydep,wetdep}}$
  - $\Delta M_{trans,chem,drydep,wetdep}$: the total mass rate of change due to transport, chemistry, deposition
  - $M$: the NH3 mass in each grid (column)
- $\tau_{mod} = \frac{M}{-\Delta M_{trans,chem,drydep,wetdep}}$

# Ammonia-water equilibrium

- $NH_3 + H_2O \rightleftharpoons NH_3 \cdot H_2O$
- $H_{NH_3} = \frac{[NH_3 \cdot H_2O]}{\mathrm{p}_{NH_3}}$, Henry's Law
- $NH_3 \cdot H_2O \rightleftharpoons NH_4^+ + OH^-$
- $K_1 = \frac{[NH_4^+][OH^-]}{[NH_3 \cdot H_2O]}$
- $[NH_4^+] = \frac{K_1 * H_{NH_3}}{[OH^-]} \mathrm{p}_{NH_3} = K_{NH_4^+/NH_3} * C_{NH_3}$
- $K_{NH_4^+/NH_3} = \frac{[NH_4^+]}{C_{NH_3}}$
- $\tau_{mod} = \frac{M_{NH_3} + M_{NH_4^+}}{-(\Delta M_{NH_3,}^{drydep,wetdep} + \Delta M_{NH_3}^{drydep,wetdep})} \rightarrow \frac{(K_{NH_4^+/NH_3}^{\mathrm{mod}} + 1) M_{NH_3}}{-\Delta M_{NH_3,NH_4^+}^{drydep,wetdep}}$

# Effective lifetime and correspond emissions

- $\tau_{mod} = \frac{(K^{\mathrm{mod}}_{NH_4^+/NH_3} + 1) M_{mod}}{-\Delta M^{drydep,wetdep}_{NH_3,NH_4^+}}$
- $\tau'_{mod} = \frac{\tau_{mod}}{K^{\mathrm{mod}}_{NH_4^+/NH_3} + 1} = \frac{M_{NH_3}}{-\Delta M^{drydep,wetdep}_{NH_3,NH_4^+}}$
- $\hat{E}_{obs} = \frac{(M_{\mathrm{obs}} - M_{mod})}{\tau'_{mod}} + E_{mod}$

# Delta Concentration

- Absolute： $C_{obs} - C_{\mathrm{mod}}$
- Relative: $\frac{|C_{obs} - C_{\mathrm{mod}}|}{C_{obs}} \times 100\%$

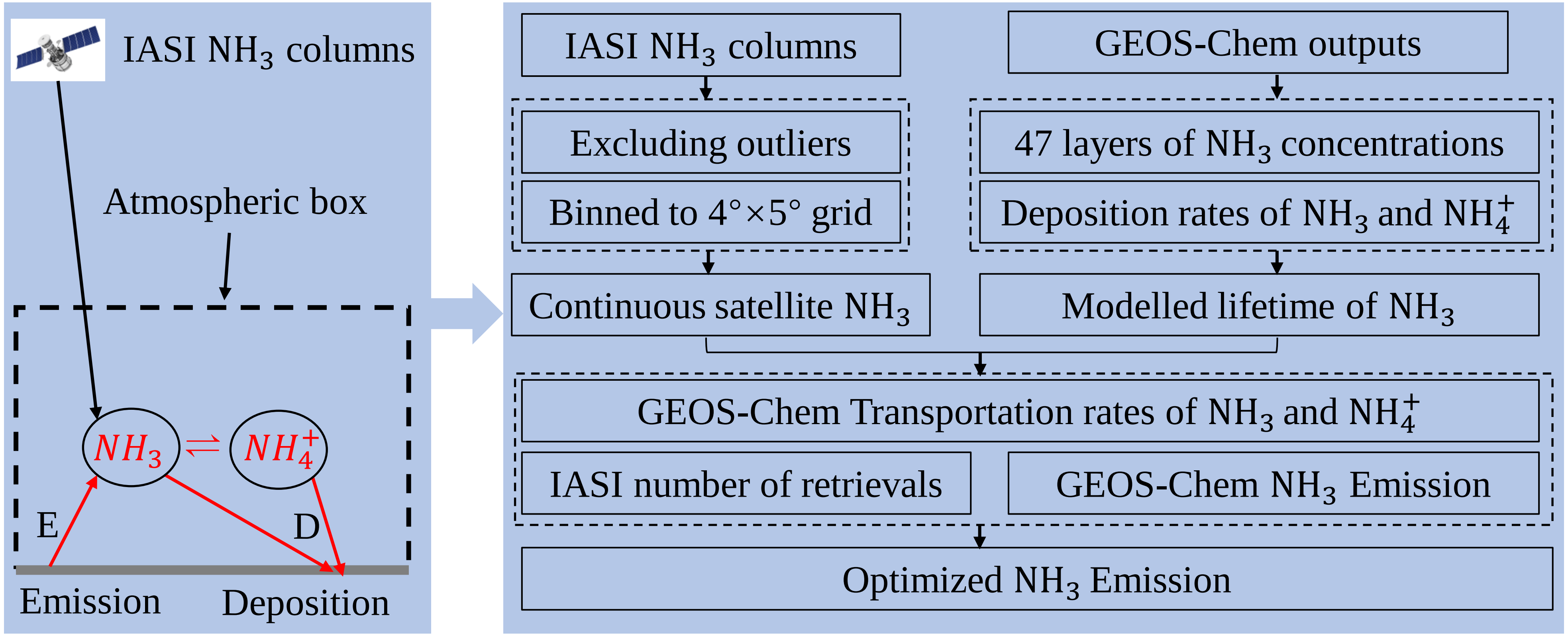
Secondary inorganic aerosols

- $2NH_3 + H_2SO_4 == (NH_4)_2SO_4$
- $NH_3 + HNO_3 == NH_4NO_3$

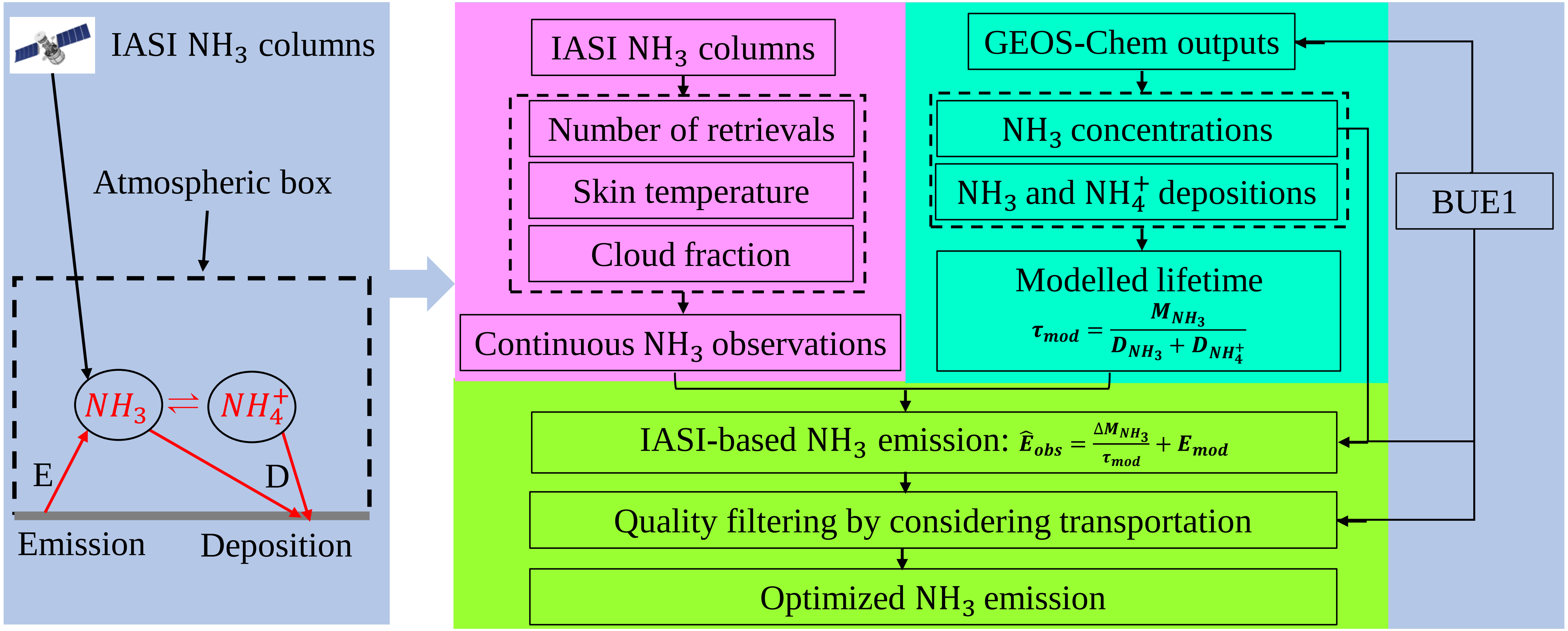
uncertainty

- $\mathrm{E}rror = \frac{relative\_error}{\sqrt{n}}$

# Diagram and Flowchart of using IASI data and GEOS-Chem simulation to optimized NH3 emission.



# Diagram and Flowchart of using IASI data and GEOS-Chem simulation to optimized NH3 emission.



# Diagram and Flowchart of using IASI data and GEOS-Chem simulation to optimized NH3 emission.