Rapid Inference of Physically-informed Top-Down Emissions using the AI-driven Inverse Model with Observations

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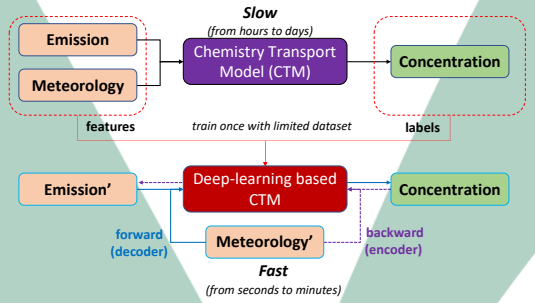
ABSTRACT

- Deterministic AI-driven CTM modeling system that can emulate the complex Community Multiscale Air Quality (CMAQ) modeling system to estimate ambient concentrations.
- Development of rapid inference of physically-informed Top-down Emissions using the AI-driven Inverse Emissions Modeling system called Variational AutoEncoder (VAE) compared to other inverse modeling techniques, such as Adjoint and Mass Balance approaches.



METHOD

Inputs (*row,column,height,time*)

- **Emissions**
  - **Sectors:** Power, industry, transport, agricultural, livestock, etc.
  - **Pollutants:** SO_2, NOx, NH3, VOC, PMs
- **Meteorology**: Temperature, WS, WD, PBL, etc.
- **Geography:** LAI, Land cover, elevation, etc.

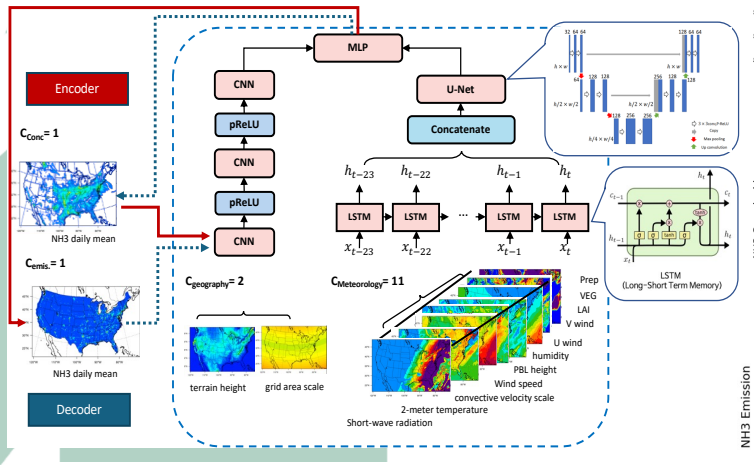
Outputs (*row,column,height,time)*

- **Pollutants:** SO_2, NO_2, O_3, VOC, $PM_{2.5}$

- *Training is required with significant computing resources to learn from high-dimensional inputs*
- *Used limited training datasets due to the limited GPUs and CPUs memories on the high-performance computing clusters*
- *A couple of minutes to run the training AI models.*

Variation AutoEncoder (VAE)

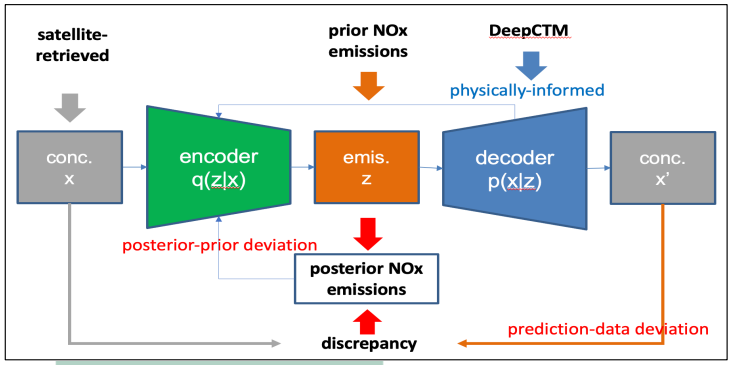
- ***VAE Decoder***: *Emissions →Concentrations*
- ***VAE Encoder***: *Concentrations →Emissions*



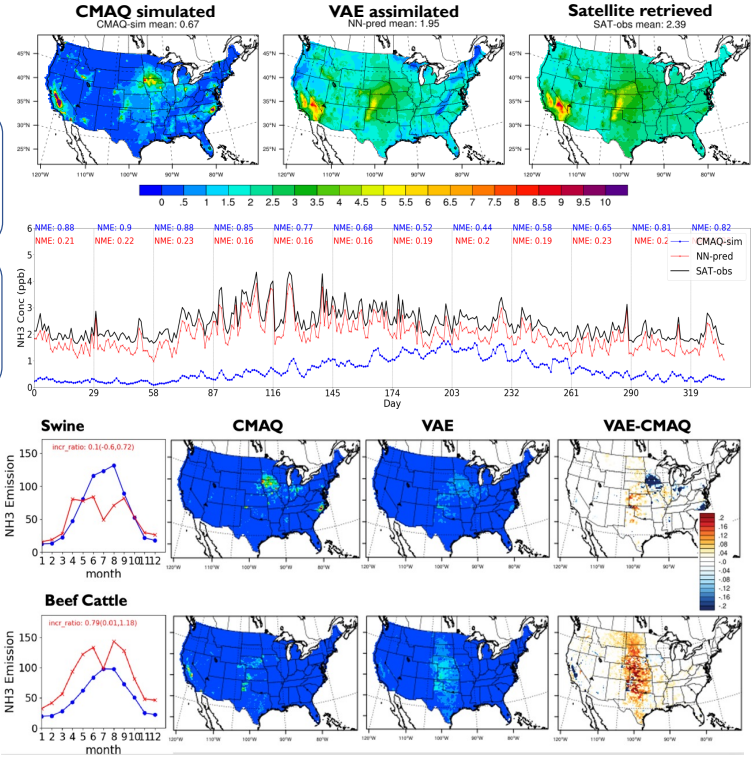
VAE Encoder Inverse Emissions System

- Trained physically-informed VAE Encoder with CTM daily concentrations and daily emissions/hourly meteorology
- **Inputs**: Seamless daily concentration maps of pollutants and hourly meteorology variables
- **Outputs**: Physically-informed top-down daily emissions

Variational AutoEncoder (VAE) ***(Xing et al., ES&T, 2022)***



RESULTS



CONCLUSIONS

- EPA's Livestock Ammonia (NH_3) emissions show spatially and temporally differences compared to VAE-top-down dailyNH_3
- EPA's static estimates are overall under-estimated compared to dynamically-estimated NH_3 with local meteorology
- EPA's static daily NH_3 emissions do not capture local meteorological impacts on their emissions.
- Animal-specific NH_3 comparison shows:
  - Over-estimation of NH_3 from Swine over IA and NC
  - Under-estimation of NH_3 from Beef cattle over the mid-U.S.
- Physically-informed top-down daily emissions can be used to guide emission's spatiotemporal patterns.
- VAE-Encoder top-down emissions rely on the quality of concentrations