

# ACOM Seminar

## Development of Spatiotemporal Physically-informed Top-Down NH<sub>3</sub> and NO<sub>x</sub> Emissions over the U.S. using an AI Machine-Learning Inverse Modeling System with Observations.

**B.H. Baek**

George Mason University

Date: Thursday, 15 February 2024, 11:00 am – 12:00 pm (MT)

Link: <https://operations.ucar.edu/live-acom>

### ABSTRACT

Timely accurate estimation of NH<sub>3</sub> and NO<sub>x</sub> emissions plays a critical role in forming PM<sub>2.5</sub> concentrations in the atmosphere. While the bottom-up method can provide an averaged value, the satellite-based top-down methods can generate near-real-time constraints on emissions; however, the existing numerical models (e.g., chemical transport model, CTM) can be computationally expensive, and its efficiency can be largely limited by efforts in dealing with the complex emission-concentration response. However, the computational burden can be significantly improved with the use of a deep neural network trained with CTM simulations, note as DeepCTM. We apply this novel machine-learning-based method (DeepCTM) using a physically informed variational autoencoder (VAE) emission predictor to infer NH<sub>3</sub> emissions from satellite-retrieved and ground-based concentrations of NO<sub>2</sub> and NH<sub>3</sub>. The VAE emission predictor has successfully implemented in NO<sub>2</sub> concentrations with the satellite-retrieved surface NO<sub>2</sub> concentrations. The proven interpretability of the VAE emission predictor will be applied using sensitivity analysis by modulating each feature, indicating that NH<sub>3</sub> and NO<sub>2</sub> concentrations and local meteorology are highly correlated for estimating NH<sub>3</sub> emissions. The advantages of the VAE emission predictor in efficiency, flexibility, and accuracy demonstrate its great potential in estimating the latest spatiotemporal emissions and its future applications.

For more information, please contact Qing Ye (qingye@ucar.edu) or Kyle Zarzana (kzarzana@ucar.edu).

The National Center for Atmospheric Research is operated by the University Corporation for Atmospheric Research under the sponsorship of the National Science Foundation