**OAQPS Pre-approval Abstract**

Author: Jim Kelly and Carey Jang

Group Leader: Tyler Fox

Division: AQAD

Date: 26 March 2021

1. What is the working title of the proposed manuscript?

Deep learning for predicting ozone variations with emissions and meteorology

1. What questions do you intend to address?

We intend to demonstrate the capability of deep learning methods for predicting ozone concentrations from emission and meteorology inputs. The study is an initial step toward the goal of developing efficient deep learning models that replicate the key features of chemical transport models (CTMs) but with increased computational efficiency compared with CTMs.

1. What methodology do you intend to use to address the questions (e.g., data, models, etc.)?

We will primarily use the CMAQ chemical transport model and a neural network modeling approach developed in our previous study.

1. What are the anticipated limitations and uncertainties associated with the proposed work?

The largest limitation is that errors in predictions of the neural network model accumulate over multiple time steps and create problems for typical model applications with long integration times. This issue is addressed in the current study by limiting simulations to a 24-hr period, but future work will be needed to address the error accumulation problem.

1. How would the proposed paper support or advance the OAQPS programmatic responsibilities? Please point to specific OAQPS actions (past, present, future) where this publication could have tangible benefits.

OAQPS assessments can be limited by the computational expense of photochemical air quality modeling. Deep learning methods have the potential to more efficiently simulate the nonlinear processes that influence ozone and PM2.5 concentrations. Once demonstrated to be accurate and reliable, deep learning approaches could provide improved information for future OAQPS actions involving modeling of the air quality impacts of different policy options.

1. With whom do you plan to collaborate as authors/co-authors (including those internal to OAQPS as well as outside of OAQPS)? Please list names and organizational affiliation. Is the envisioned authorship complete and appropriate? Please explain briefly.

This study is led by our colleagues at Tsinghua University. This project is part of our long-standing collaboration with the ABaCAS (Air Benefit and Cost and Attainment Assessment System) team on developing efficient tools for air quality management. The author list (envisioned complete) is as follows:

Jia Xing1,2, Shuxin Zheng3, Siwei Li4, Xiaochun Wang1,2, James T. Kelly5, Shuxiao Wang1,2, Yueqi Jiang1,2, Song Liu1,2, Chang Liu3, Carey Jang5, Yun Zhu6, Tie-Yan Liu3, Jiming Hao1,2

1 State Key Joint Laboratory of Environmental Simulation and Pollution Control, School of Environment, Tsinghua University, Beijing 100084, China

2 State Environmental Protection Key Laboratory of Sources and Control of Air Pollution Complex, Beijing 100084, China

3 Microsoft Research Asia, Beijing 100080, China

4 School of Remote Sensing and Information Engineering, Wuhan University, Wuhan 430079, China

5 Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, NC 27711, USA

6 College of Environment and Energy, South China University of Technology, Guangzhou Higher Education Mega Center, Guangzhou 510006, China

1. Who is the audience? And what key messages do you anticipate communicating to audience?

The primary audience is the air quality modeling community and users of reduced-form modeling techniques. The key message is that deep learning has the potential to improve the efficiency of photochemical air quality modeling, but technical barriers remain and more development is needed.

1. Abstract (brief)

Fast and accurate prediction of ambient ozone (O3) responses to changes in emissions and meteorology is crucial for designing effective pollution control strategies. However, existing chemical transport model (CTM) approaches are computationally expensive, and this expense limits their usage. Here we proposed a novel method (noted as DeepCTM) that applies deep learning to CTM predictions to improve the computational efficiency of photochemical modeling. The well-trained DeepCTM successfully reproduces CTM-simulated O3 concentrations using input features of precursor emissions, meteorological factors, and initial conditions. The advantage of the DeepCTM is its high efficiency in identifying the dominant contributors to O3 formation and quantifying the O3 response to variations in emissions and meteorology. The DeepCTM application in China suggests that O3 concentrations are strongly influenced by the initialized O3 and NO2 concentrations, as well as emission and meteorological factors during daytime when O3 is formed photochemically. The DeepCTM developed in this study exhibits great potential for efficiently representing the complicated atmospheric system and in the future may inform policy makers in designing effective control strategies to mitigate the O3 pollution.