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Proposal title: Improved emissions and oxidation mechanisms for non-transport VOC emissions in air quality forecasting models

PI: Kelvin Bates, Assistant Professor, Department of Mechanical Engineering, University of Colorado Boulder; **Co-I**: Deepangsu Chatterjee, graduate student, Washington University in St. Louis (joining University of Colorado Boulder as a postdoc). **Collaborators:** Researchers in NOAA CSL's Tropospheric Chemistry & Atmospheric Composition Modeling groups.

Competition: This proposal falls under Air Quality Research & Forecasting, specifically addressing priority areas AQRF-2 (evaluation of the NAQFC system), AQRF-3 (improved spatial and temporal emission estimates), and AQRF-7 (optimization of chemistry processes).

Background: Accurately predicting concentrations of atmospheric ozone and particulate matter, the two most harmful criteria pollutants, requires a precise knowledge of the spatial and temporal pattern of emissions of volatile organic compounds (VOCs) to the atmosphere and the chemistry by which those VOCs react. In previous decades, urban VOCs in the US were dominated by emissions from fossil fuel use in the transportation sector, for which atmospheric reactivity and emission inventories could be precisely calibrated. As regulatory measures caused decreases in VOC emissions from vehicles and their associated fossil fuel infrastructure, the relative importance of other, more diffuse VOC sources such as cooking, volatile chemical products (VCPs), and urban vegetation have increased.[1,2] These emission sources are not well represented in current inventories, and the specific VOCs they emit are frequently not treated explicitly in model mechanisms, leading to difficulties in the accurate prediction of ozone and particulate pollution events and in the assessment of potential emission reduction strategies' efficacies.

We propose to use newly collected data sets from NOAA CSL field studies in major US urban areas to develop, assess, and optimize improved emission inventories and reduced chemical mechanisms for VOCs from the VCP, cooking, and urban vegetation sectors. These inventory and mechanism modules will then be integrated into UFS-Chem, NOAA's air quality forecasting model under development, to improve model representation of non-transport VOC sources and their impact on air quality, and the model will be assessed against field data. We recently participated in NOAA's SUNVEx, AEROMMA, and USOS campaigns, on which extensive field data sets of VOCs and air pollutants were collected across the US. Box modeling of these data have already helped us to identify important emission sources and key VOCs not previously implemented in models, construct preliminary inventories of their emissions, and test simplified mechanisms of their oxidation.[2-5] Funding for this proposal will allow us to optimize and finalize these inventory and mechanism modules, consolidate them into UFS-Chem, assess their impact on model bias, and make them available for researchers, air quality forecasters, and other users. We will also use these outputs to simulate emission reduction strategies in US urban areas.

Planned products & outputs: The major products of this proposed research will include (1) comprehensive, validated emission inventories of VOCs from key non-transport urban sectors, including VCPs, cooking, and urban vegetation, with temperature, diurnal, and seasonal variability, which will both be implemented into NOAA's UFS-Chem model and made available as modules more other models; and (2) reduced chemical oxidation mechanisms to account for the atmospheric impacts of key VOCs from these new inventories, also integrated into UFS-Chem and made available for other models such as GEOS-Chem, F0AM, and CMAQ.

Planned impacts, benefits, & outcomes: The deliverable outputs from this proposed research plan (inventories and mechanism modules) will improve UFS-Chem representation of air quality outcomes. They will also improve the temperature, diurnal, and seasonal sensitivities of air quality forecasts, as these dependences will be integrated into the inventories, and their sensitivity to changes in specific sectoral emissions. Our own simulations as part of this research will demonstrate the relative efficacy of emissions

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reductions across various sectors in US urban areas, to better understand the contributions of individual sectors to poor air quality outcomes, which can in turn inform policymakers about optimal pollution control strategies. Future users of both UFS-Chem and the other models in which we make our modules available will also benefit from the improved capabilities that come with these optimized modules.

Planned methodology & timelines: Initial formulation of inventories and mechanisms have already been demonstrated, but testing has been performed in disparate test beds (various model frameworks, mostly box modeling) and often against non-US data.[5-6] Our first task will be to compile the VCP, cooking, and urban biogenic inventories into a single module deployable in both GEOS-Chem and UFS-Chem, and to consolidate the mechanism development from GEOS-Chem and box models. In the first and second years, temperature, diurnal, and seasonal dependences will be tested in the emission inventories, and additional simplifications tested in the mechanisms to minimize computational cost to end users. After optimizing both modules, in the second and third year their implementation in UFS-Chem will be further validated against field data collected across the US, including past NOAA campaigns and the upcoming AiRMAPs campaign, and module integration will be finalized for other UFS-Chem users. In the final year, simulations will be performed to test the air quality outcomes of specific sectoral VOC emission reduction strategies using the newly developed modules.

Starting & ending readiness levels: We assess that the prototype emission inventories and chemical mechanisms for VOCs from VCPs and cooking are at Readiness Level 5, having been tested in GEOS-Chem and box models against existing field datasets. The groundwork has already been laid for comparisons to further NOAA field measurements (for which data have been processed) and optimizing emission fields and mechanism details in GEOS-Chem. After translating the results to UFS-Chem, we expect to bring our inventories and mechanisms to Readiness Level 8, a stage at which they will be fully implemented in UFS-Chem and ready for broader-scale applications by the UFS-Chem user base.

Potential adopters of outputs: We expect the inventories and mechanisms developed herein to be broadly usable by all adopters of UFS-Chem. This will include applications to forecasting of air quality by NOAA, applications to scientific investigation by researchers at NOAA and beyond, and applications to policymakers in that the modular inventories will enable testing of potential emission reduction strategies' impacts on air quality. By making the inventories and mechanisms modular and easily integrated into other models (including GEOS-Chem, in which initial testing has been conducted, and the EPA's CMAQ model, for which the PI serves on the mechanism development team), we will also make these outputs adoptable by users of other air quality forecasting models.

Budget table: (numbers include approximate overhead and salary fringe costs)

Category	Year 1	Year 2	Year 3	Total
Salaries:				
Co-I (postdoc)	$120000	$120000	$120000	$360000
Graduate student (1.5x)	$120000	$120000	$120000	$360000
PI (fractional)	$20000	$20000	$20000	$60000
Conference travel	$6000	$12000	$12000	$30000
Publications	--	$15000	$15000	$30000
Computing resources	$10000	$10000	$10000	$30000
Total	$276000	$297000	$297000	$870000

Citations:

[1]McDonald *et al.*, 2018, DOI: 10.1126/science.aaq0524; [2]Coggon *et al.*, 2024, DOI: 10.5194/acp-24-4289-2024; [3]Coggon *et al.,* 2021, DOI: 10.1073/pnas.2026653118; [4]Gkatzelis et al., 2021, DOI: 10.1021/acs.est.0c05467; [5]Stockwell *et al.,* 2024, DOI: 10.5194/egusphere-2024-1899; [6]Travis *et al.*, 2024, DOI: 10.5194/egusphere-2024-951.