MUSICActivities

NCAR ACOM

Newsletter

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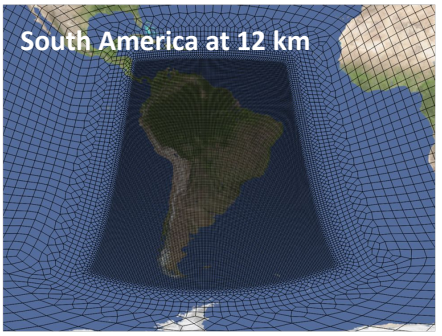
of the Multiscale Infrastructure for Chemistry and Aerosols - MUSICA

MUSICA is a computationally feasible global modeling framework currently in development that allows for the simulation of large-scale atmospheric phenomena, while still resolving chemistry at emission and exposure relevant scales (down to 4 km).
MUSICA will replace and extend the current community chemistry modeling efforts at NCAR (e.g., WACCM, CAM-Chem, WRF-Chem) paralleling other activities at NCAR to streamline and unify model developments.

Summary of this issue



New! MUSICA Library Release Version is available at https://github.com/NCAR/musica

MUSICAv0 is an initial configuration based on the CESM Community Atmosphere Model with chemistry using the Spectral Element with Regional Refinement dynamical core.

MusicBox is a box model using a model independent chemistry module.

MELODIES is a modular framework to compare model results with observations.

MUSICA is part of **SIMA** (System for Integrated Modeling of the Atmosphere).

To contribute to the newsletter, please email alma@ucar.edu

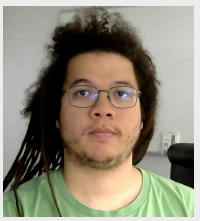
Toward Emulating an Explicit Organic Chemistry Mechanism With Random Forest Models

Contributed by **Camille Mouchel-Vallon** *(camille.mouchel-vallon@aero.obs-mip.fr)*
Laboratoire d'Aérologie, Université de Toulouse, CNRS, UPS, Toulouse, France

In short

Organic compounds constitute a significant fraction of atmospheric particles and thus have an impact on health and climate. Predicting the contribution of organic compounds to atmospheric particles is extremely complex because of the very large number of different chemical species potentially condensing into the aerosol phase. Air quality and climate models usually rely on simplified, empirical approaches to predict organic aerosol mass concentrations, based on laboratory experiments. In this work, we apply a machine learning approach to construct a tool that behaves like the most detailed organic chemistry model, for a numerical cost affordable by air quality and climate models.

Camille Mouchel-Vallon



Camille is currently a postdoc fellow at the University of Toulouse, France. He worked at NCAR for three years till 2020.

Camille's research focuses on improving and applying detailed organic chemistry mechanisms such as GECKO-A to further our understanding of aerosol formation and properties. He is also involved in model evaluations using field campaign measurements.

Findings

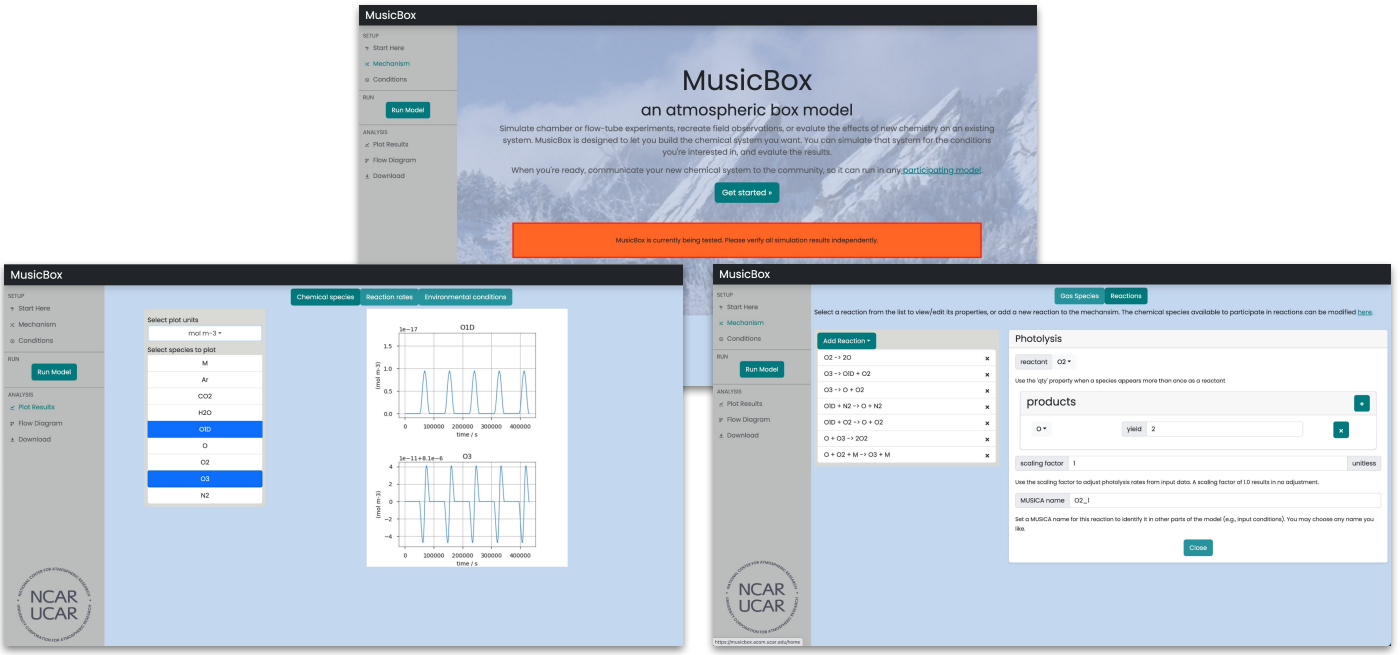
Recurrent random forests were trained to predict organic matter formation from dodecane and toluene precursors, and its partitioning between gas and particle phases. Validation tests show that the random forests perform well without any divergence over 10 days of simulations compared with a fully explicit chemical model GECKO-A. We also found that the most important predictors are those providing information about the chemical regime, oxidants levels, and existing organic mass. The choice of predictors is crucial as using too many unimportant predictors reduces the performances of the random forests. The use of this emulator offers a remarkable computational speedup of 100 to 100,000 times compared to the computationally intensive traditional models.

Mouchel-Vallon, C., & Hodzic, A. (2023). Toward emulating an explicit organic chemistry mechanism with random forest models. Journal of Geophysical Research: Atmospheres, 128, e2022JD038227.

MusicBox Interactive

An interactive box model in your web browser!

ACOM introduces MusicBox, an interactive box model that allows users to explore various chemical gas-phase mechanisms. Developed by our dedicated student interns, MusicBox features an impressive interface that enables interactive modeling. Users can easily prescribe simulation conditions and interactively explore the results.



- **MusicBox Interactive is live!**

Navigate to musicbox.acom.ucar.edu or scan the QR code to be taken to the site. Instructions for using the model can be found on the home page. Please be aware that the site and model are still being tested and verified. If you find an issue or have an idea for a new feature, let us know at github.com/NCAR/music-box-interactive-client/issues!

Special thanks to our amazing interns Simon Thomas, Jordan Wood, Julien King, and our partners at the University of Illinois Urbana-Champaign for their efforts!

MUSICA Library Release

Checkout updates to the various components that make up the MUSICA library below! The MUSICA library will comprise all the aerosol and chemistry modules developed as part of the MUSICA project.

MUSICA Library Release Version 0.3.0

- Repository: https://github.com/NCAR/musica

- Highlighted features or updates
  - Includes updated TUV-x, MUSICA-Core, and MICM versions
  - Connections to CAM-SIMA for MUSICA have been started to allow early adoption of the MICM solver when MICM is completed.

TUV-x Version 0.5.0

- Repository: https://github.com/NCAR/tuv-x

- The TUV-x photolysis calculator is a runtime-configurable tool that calculates photolysis rate constants and diagnostic dose rates using standardized input data. The tool accepts user-provided radiation fields, or calculates them using the Delta-Eddington or n-Stream methods. The tool can be used as a stand-alone executable or through an API, and can be embedded in a 3D atmosphere model for added flexibility.

- Highlighted features or updates
  - Fixed a bug where the profiles read from a configuration file for radiation was improperly setup.

MUSICA-Core Version 0.3.0

- Repository: https://github.com/NCAR/musica-core

- MUSICA-Core is a collection of common utilities and algorithms needed by MUSICA software bundled into a single library. This library is agnostic of the model it is used in, but crucially is designed to allow runtime configurability of each of our models.

- Highlighted features or updates
  - Added the ability to append to output file variables.

MUSICA Library Release

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Music Box Interactive 2.0.0

- Repository: https://github.com/NCAR/music-box-interactive
- Highlighted features or updates
  - Hosted service with multi-user capabilities

MICM 3.1.0

- Repository: https://github.com/NCAR/micm
- Highlighted features or updates
  - Includes a hard-coded gas-phase solver for the Chapman mechanism, the beginnings of a general purpose Rosenbrock solver for any gas phase mechanism, parsing of CAMP configuration files, and scaffolding to support GPU-enabled chemistry.

CAMP 1.1.0

- Repository: https://github.com/open-atmos/camp
- Highlighted features or updates
  - Added support for condensed phase photolysis and surface reaction reaction types.

CAM-SIMA

The Community Atmosphere Model (CAM) is currently being rewritten to accommodate infrastructure needs of the Common Community Physics Package (CCPP), referred to as CAM-SIMA. CCPP will allow for easy interoperability with other physics and chemistry packages, enabling users to configure their simulations for global to regional to local scale applications representing the dynamics, physics, and chemistry most appropriate for the science question. CAM-SIMA is slated to replace CAM in the future. For more information about SIMA, see https://sima.ucar.edu/

Workshop Presentations and Publications

CESM 2023 Workshop, Boulder

https://www.cesm.ucar.edu/events/162/agenda

- **Mary Barth,** Update on the System for Integrated Modeling of the Atmosphere (SIMA)
- **Louisa Emmons,** Modeling Air Quality with Variable Resolution in CESM
- **Noribeth Mariscal,** Evaluation of Ozone and its Precursors Using Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) during the Michigan-Ontario Ozone Source Experiment (MOOSE)
- **Duseong Jo,** Comparison of urban air quality simulations during the KORUS-AQ campaign with regionally refined vs global uniform grids in the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) Version 0

Joint WRF/MPAS Users Workshop 2023, Boulder

https://www.mmm.ucar.edu/events/workshops/wrf-mpas

- **Mary Barth,** Developing the next generation chemistry modeling with MUSICA, the Multiscale Infrastructure for Chemistry and Aerosols

Publications

- Jo, Duseong, et al., Effects of Grid Resolution and Emission Inventory on Urban Air Quality Simulation with the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) Version 0, Journal of Advances in Modeling Earth Systems, https://doi.org/10.1029/2022MS003458, 2023.
- Tang, W., Emmons, L. K., Worden, H. M., Kumar, R., He, C., Gaubert, B., Zheng, Z., Tilmes, S., Buchholz, R. R., Martinez-Alonso, S.-E., Granier, C., Soulie, A., McKain, K., Daube, B., Peischl, J., Thompson, C., and Levelt, P.: Application of the Multi-Scale Infrastructure for Chemistry and Aerosols version 0 (MUSICAv0) for air quality in Africa, Geosci. Model Dev. Discuss. [preprint], https://doi.org/10.5194/gmd-2023-50, in review, 2023.