Development of the Configurable ATmospheric Chemistry (CATChem) model and its application within the Unified Forecast System forming a unified UFS-Chem

Collaborative effort between NOAA ARL, NOAA CSL, NOAA GSL, and NCAR

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Current Structure of the UFS for Atmospheric Chemistry and Composition

<table>
<thead>
<tr>
<th>Model</th>
<th>Chemistry Available</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>RRFS – Smoke/Dust</td>
<td>Simplified Aerosols: Smoke + Dust tracers</td>
<td>Regional Wildfire Smoke Forecasts</td>
</tr>
<tr>
<td>UFS - Aerosols</td>
<td>Simplified Aerosols: GOCART</td>
<td>Global Weather Forecasts with aerosol feedbacks</td>
</tr>
<tr>
<td>Online CMAQ</td>
<td>Complex chemistry from CMAQ: Ozone and Aerosols</td>
<td>Regional Air Quality Forecasts</td>
</tr>
<tr>
<td>UFS-RAQMS</td>
<td>Simplified chemistry with data assimilation: Ozone and Aerosols</td>
<td>Global air quality forecasts</td>
</tr>
</tbody>
</table>

Problems:

- Chemistry-related code is duplicated across the UFS, which is not unified and time intensive to maintain.
- The reliance on multiple externally developed models also limits expertise within NOAA.
- We would like to add research capabilities for atmospheric composition and chemistry, but it is unclear how to do this with chemistry divided across so many models/applications.
Overall Unifying Goals

- Add, update, and advance chemical and aerosol processes in the operational forecasts in order to
  - Improve aerosol feedbacks in weather forecasts
  - Improve aerosols in wildfire smoke forecasts
  - Improve ozone and aerosols in air quality forecasts
- Add enhanced research capabilities including more complex chemistry, aerosol, and physics options in order to improve operational forecasts indirectly or on longer timescales by
  - Collaborating more with the research community
  - Advancing current understanding of air quality and atmospheric composition processes
- **Unite** together across all of NOAA and in the community to advocate for the importance of adding aerosols and chemistry for accurately representing processes in the operational forecast models
  - A simple aerosol scheme is needed in the UFS weather model
  - Smoke & dust tracers are needed for wildfire smoke operational forecasts
- **In order to accomplish these goals, we need to unify chemistry in the UFS (UFS-Chem)**
  - OAR laboratories use and develop UFS-Chem for research and R2O activities
  - EMC uses and develops UFS-Chem for operational forecasts and O2R activities
  - We jointly work together to advocate for the importance of including aerosols and chemistry within the UFS

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Unify Chemistry across the UFS through CATChem development

We propose to develop a chemistry package/library, which will be a submodule of the ufs-weather-model and store all chemistry related code in one unified location.

- **Src**: Stores all chemistry related process level source code for the UFS
- **Parameters**: Stores all chemistry and aerosol information in tables
- **Util**: Stores all tools and utility functions related to chemistry
- **Drivers**: All files needed to link UFS - Chem to the UFS
- **CCPP**: Possibly other models in the future
- **NUOPC**: Possibly other models in the future
Options to use gas & aerosol chemistry of varying complexity

CATChem

Aerosol Schemes
- None
- Smoke + dust tracers
- GOCART
- ISORROPIA (CMAQ)

Gas-phase chemical mechanisms
- None
- Greenhouse gas tracers
- REDHC - RAP-Chem
- Carbon Bond (CMAQ)
- Complex research mechanisms

Increasing complexity & computational cost

UFS-Chem will be flexible and configurable where users can choose the aerosol scheme and the gas-phase chemical mechanism of the right complexity for their desired application or science question
Options to use gas & aerosol chemistry of varying complexity

- CATChem
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    - None
    - Smoke + dust tracers
    - GOCART
    - ISORROPIA (CMAQ)
  - Gas-phase chemical mechanisms
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- RRFS-Smoke/Dust
- UFS - Aerosols
- Online CMAQ
- Research questions (e.g., addressing new emerging emissions sources)
- New applications for connections to climate
This overall structure is similar to how the land model is configured and coupled to the UFS.

Blue boxes are git submodules. Gray boxes are folders within git submodules. White boxes are description of the files in a given folder.

util

Tools and utility functions that are not part of the workflow, but still potentially helpful for users (e.g., preprocessing scripts for setting up different configurations or post-processing scripts for linear interpolation)

ccpp

All files needed to link UFS-Chem through ccpp-physics (e.g., all wrapper files)

nuopc

All files needed to link UFS-Chem through nuopc (e.g., all files for NUOPC cap)
All code needed for calculations relevant to gases and SOA (e.g., MDA8 output, code to translate gas-phase SOA precursors to aerosol schemes, code to translate chemical tables in parameters section to MICM, etc.)

All code needed for calculations relevant to aerosols (e.g., PM2.5 output, calculating aerosol optical properties, etc.)

Add code to incorporate chemical and initial conditions including regridding to the UFS model.
For each mechanism, create a subfolder that includes tables (format TBD) of all reaction rates, chemical species information, mapping files to emissions, mapping files to photolysis rates, mapping files to initial and boundary conditions.

For each aerosol scheme, create a subfolder that includes tables of all aerosol properties, mapping files to emissions, mapping files to initial and boundary conditions, & mapping to calculate output (e.g., PM2.5).

Template files defining the reaction rates available for each photolysis scheme.

Template files defining the species available for each emissions dataset.

Template files defining the species available for each initial/boundary conditions dataset.

Add small files for stagnant boundaries (e.g., monthly climatology).
Model Independent Chemistry Module (MICM)

- Use MICM, which is a component of the MUlti-Scale Infrastructure for Chemistry and Aerosols (MUSICA), led by NCAR (https://github.com/NCAR/micm)
- By collaborating with NCAR on MICM development, chemistry developments from the research community incorporated into MICM will be efficiently linked to both NOAA and NCAR models.
NOAA Emissions and eXchange Unified System (NEXUS)

Aerosols

Anthropogenic & Biofuel

Biomass Burning

Historical & Future Projections (IPCC, RCP)

Extensions (Dust, Sea-Salt Biogenic, etc.)

Anthropogenic Aircraft & Ship

Non-Emission Data (Satellite O₃, LAI, Albedo, etc.)

Natural Sources

Halogens

Emissions Processing System for NOAA’s UFS Atmospheric Composition Models

Model-Ready Emissions Data

Operations

Research

C. A. Keller et al.: Emission component HEMCO

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Goals of CATChem in the UFS

- Initial code repository is created, [https://github.com/ufs-community/catchem](https://github.com/ufs-community/catchem)
- Simplify maintenance and increase efficiency in code development
  - Reduction of libraries (e.g., MAPL and related libraries)
- Unify atmospheric composition & chemistry modeling in the UFS by creating a flexible system that can be used for a variety of applications
  - All chemistry related code is stored in one location
  - Enhance collaborations between OAR laboratories for research
  - Enhance collaborations between EMC and OAR to advance R2O and O2R activities
  - Reduces costs for transitioning research advances to operations
  - Engage the research community in development by positioning the UFS as a state-of-the-art modeling system for simulating atmospheric composition across regional to global scales
- Unify emission processing with NEXUS across applications
  - [https://github.com/noaa-oar-arl/nexus](https://github.com/noaa-oar-arl/nexus)
- Continue to develop MELODIES MONET - unifies model evaluation activities
  - [https://github.com/noaa-csl/melodies-monet](https://github.com/noaa-csl/melodies-monet)
  - [https://github.com/noaa-oar-arl/monetio](https://github.com/noaa-oar-arl/monetio)
  - [https://github.com/noaa-oar-arl/monet](https://github.com/noaa-oar-arl/monet)