Experimental Air Quality Forecasting with the Rapid-Refresh Model Coupled to Chemistry (RAP-Chem)

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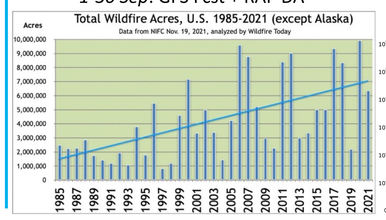
Abstract

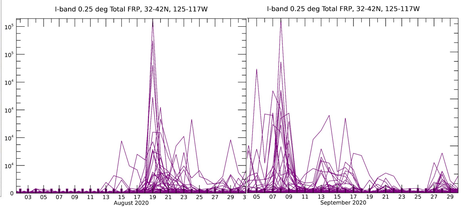
Experimental air quality forecasts with the Rapid-Refresh model coupled to chemistry (RAP- Chem) at NOAA ESRL began in July 2020 in an effort to capture changing atmospheric composition due to the emissions reductions associated with the COVID-19 lockdowns. The full gas-phase and aerosol chemistry mechanism used in the RAP-Chem and proposed for transition into the Unified Forecast System (UFS) offers a potential lower computational cost alternative compared to mechanisms used in similarly capable operational models. Additionally, the RAP-Chem includes wildfire emissions of gases and aerosols, natural emissions of biogenic gases, dust, and sea salt, and simulates aerosol feedback to atmospheric physics allowing evaluation of the impact of changes in atmospheric composition on numerical weather prediction and feedbacks on air quality. Here we will show results of retrospective forecasts of the August-September 2020 wildfire season to highlight key model features and developments in the RAP-chem that are slated for potential implementation into the UFS; specifically, we will demonstrate the suitability of a reduced complexity gas-phase chemical mechanism and its coupling to a VBS-SOA aerosol module, the improvements associated with the use of inline non-local mixing of chemical species with the MYNN PBL scheme, and coupling of the full TUV photolysis module.

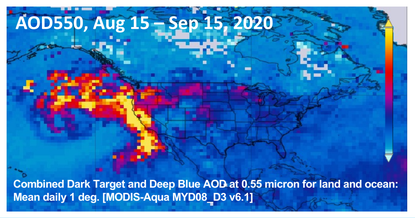
Motivation and Retrospective Simulations

- Initialized 29 July 2020 with default WRF-Chem chemical profiles (i.e., "clean")
- **Two periods**:
  - *1-31 Aug*: forced with GFS Analysis
  - *1-30 Sep*: GFS Fcst + RAP DA
- **Two simulations:** with and without aerosol (direct) feedback
- **Wildfire** and heat wave periods
- Primary analysis for August 2020

- **Can a reduced complexity chemical mechanism compete with state-of-the-science, complex mechanisms?**
- **Does improved physics/chemistry coupling improve AQ and weather forecasts?**
- **Can this modeling system accurate simulate AQ during exceptional events (e.g.,O_3 and PM from wildfires)**

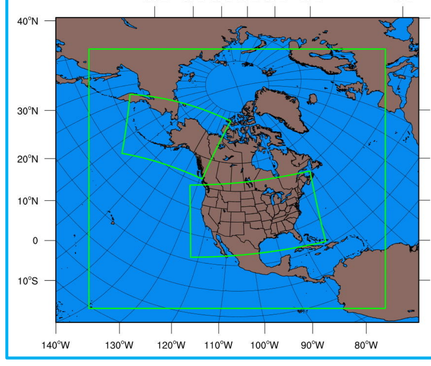




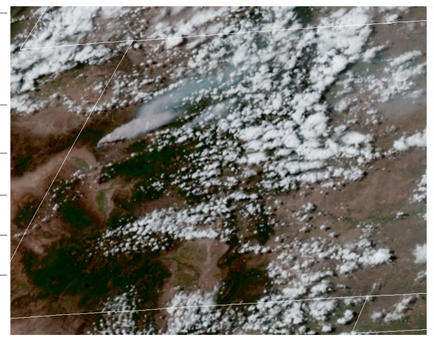


RAP-Chem real-time workflow

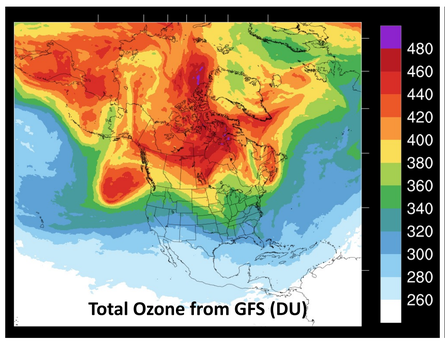
1) The **Rapid-Refresh** (RAP, *domain outer green, with nested HRRR*) model cycles hourly. We use the 06Z and 18Z forecast's ICs & BCs, taking advantage RAP's DA.



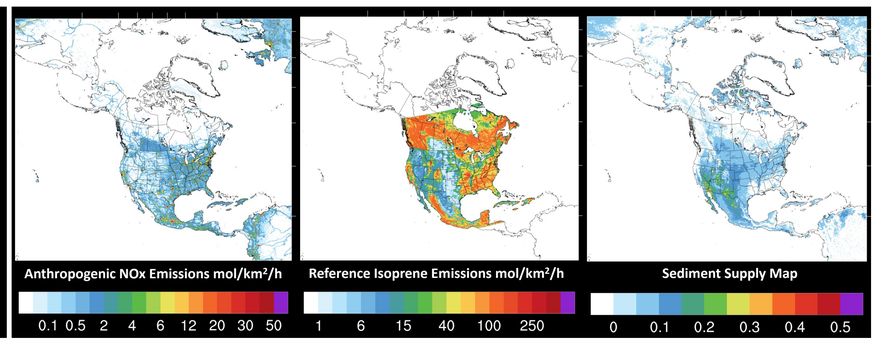
2) Remotely-sensed fire radiative power (FRP) is used to create emissions over the domain and speciated to the chemical mechanism used in RAP-Chem



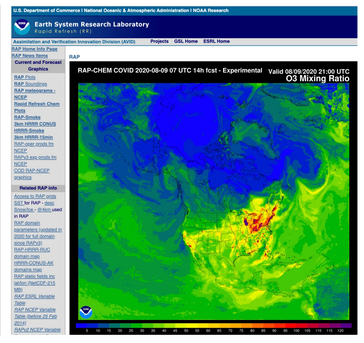
3) Total ozone columns from the real-time GFS forecast are ingested for more accurate photolysis rates and chemical BCs are ingested from the RAQMS global CTM



4) Previous forecasts' chemistry and land surface fields are cycled; season and day-specific emission related data for anthropogenic, biogenic, and dust are loaded into the input file (pollen forecasts starting May 1, 2022). Model integration begins and takes ~4 hours on 666 cores.

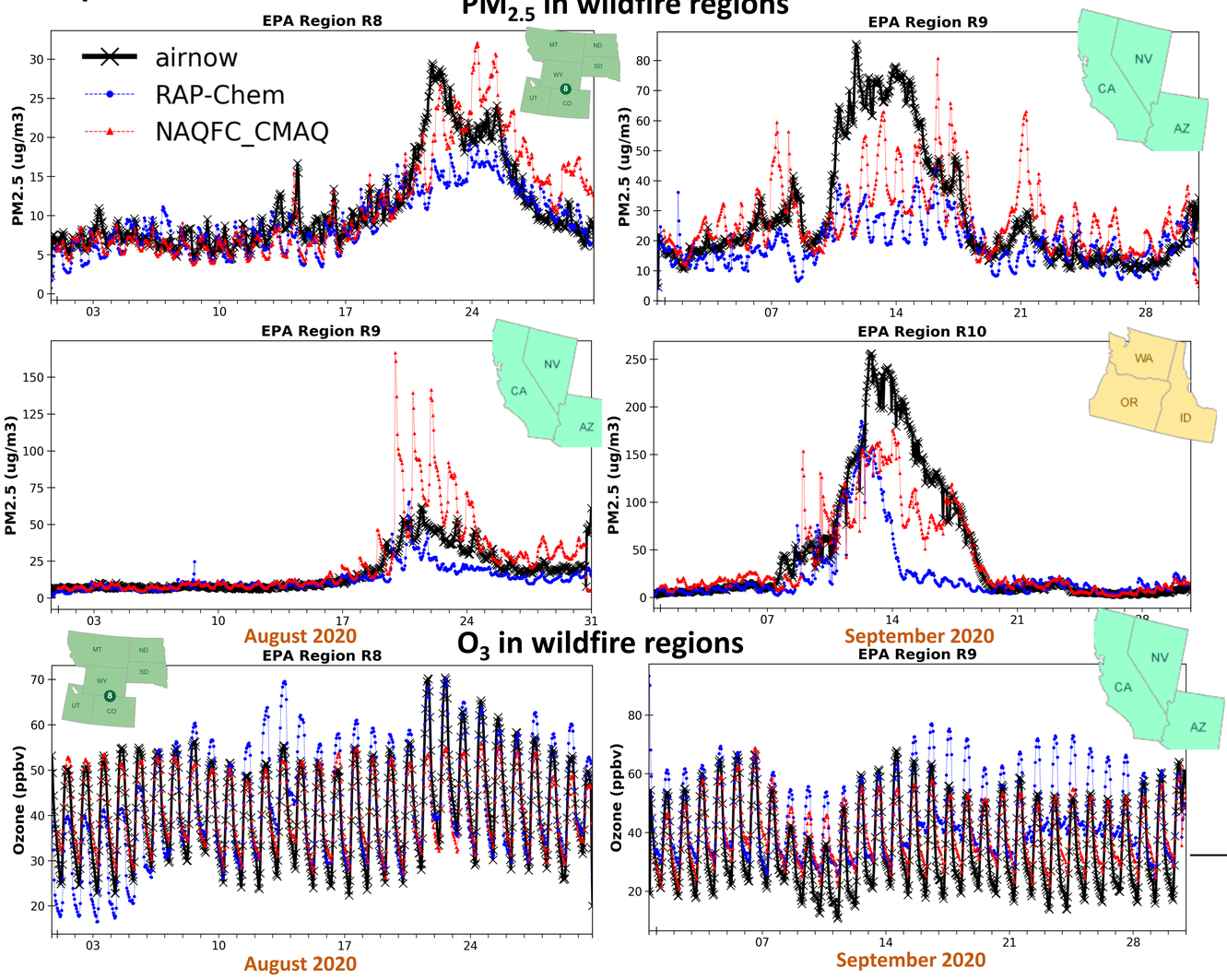


5) As model integrates, plots are published to (https://rapidrefresh.noaa.gov/RAPchem/) and subsetted data is made available to collaborators via GSL's FTP server



Results

Compare RAP-Chem to NAQFC $PM_{2.5}$ in wildfire regions



O_3 in wildfire regions

- Overall, RAP-Chem tends to outperform NAQFC for $PM_{2.5}$ in wildfire regions, though it does underestimate peak concentration days.
- NAQFC tends to outperform RAP-Chem for $PM_{2.5}$ predictions outside of wildfire impacted regions.
- For O_3, the reverse tends to be true, with RAP-Chem outperforming NAQFC in most non-wildfire impacted regions.
- In most cases, RAP-Chem simulations that includes aerosol effects on radiation/photolysis outperform those that neglect it.

Skill in all regions

AUGUST 2020

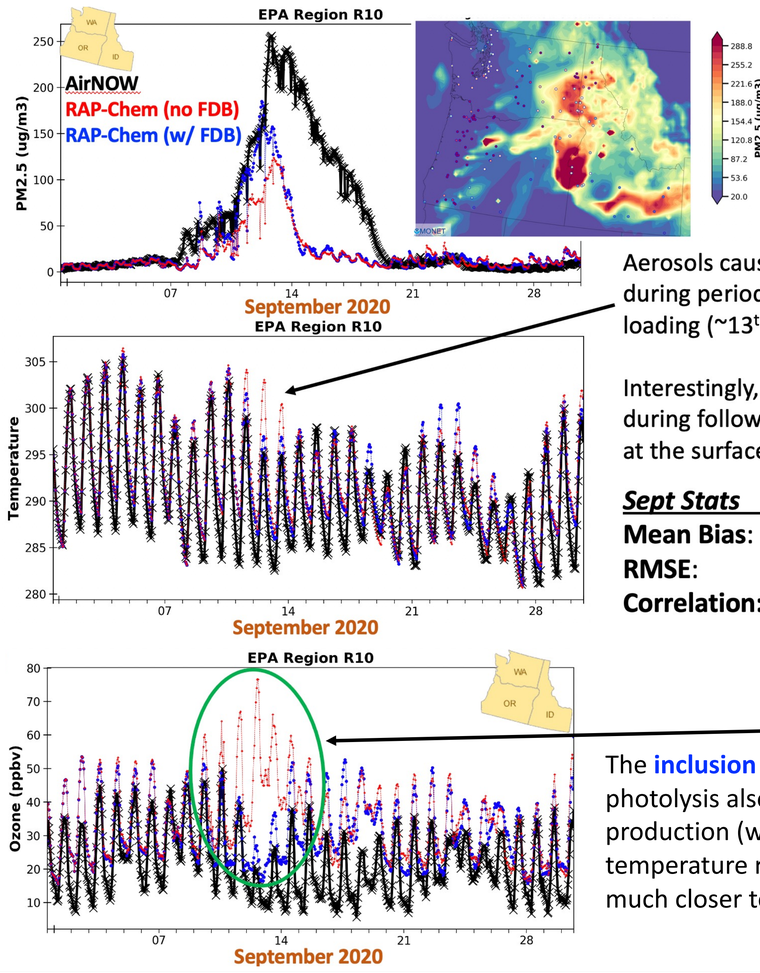
Ozone (RMSE)	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10
RAP-Chem (noFDB)	10.8	11.6	11.6	14.3	10.0	13.4	9.6	14.0	19.2	12.4
RAP-Chem (w/ FDB)	**10.4**	**11.3**	**11.4**	**14.0**	**9.6**	**13.1**	**9.0**	13.6	18.5	13.2
NAQFC	12.8	14.0	13.5	16.2	12.2	15.4	10.3	**10.9**	**14.1**	**9.9**

$PM_{2.5}$ (RMSE)	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10
RAP-Chem (noFDB)	6.2	23.5	11.9	9.6	9.9	8.1	11.9	10.4	36.4	7.9
RAP-Chem (w/ FDB)	6.1	24.3	12.0	9.3	**9.4**	7.9	11.5	**9.9**	**35.9**	**7.5**
NAQFC	**5.4**	**9.8**	**7.0**	**7.9**	10.8	**7.3**	**10.7**	10.8	60.2	10.6

September 2020

Ozone (RMSE)	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10
RAP-Chem (noFDB)	13.2	13.1	12.9	14.1	**10.7**	12.4	**9.8**	16.2	22.0	21.7
RAP-Chem (w/ FDB)	12.7	**12.4**	**12.4**	**14.0**	10.8	**11.9**	10.1	14.6	20.6	16.6
NAQFC	**11.7**	12.6	12.9	15.1	11.1	13.8	10.2	**9.9**	**15.6**	**13.8**

$PM_{2.5}$ (RMSE)	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10
RAP-Chem (noFDB)	9.9	29.8	18.0	12.3	14.8	12.9	21.5	23.8	53.7	92.7
RAP-Chem (w/ FDB)	10.7	24.2	18.7	12.0	15.6	12.5	22.0	**21.8**	**56.3**	104.9
NAQFC	**5.3**	**8.3**	**7.2**	**7.7**	**10.2**	**9.1**	**10.6**	25.7	59.4	**92.7**



Aerosol impacts on temperature forecast

Aerosols cause ~5°C temperature decrease during period with highest surface aerosol loading (~13th-14th)

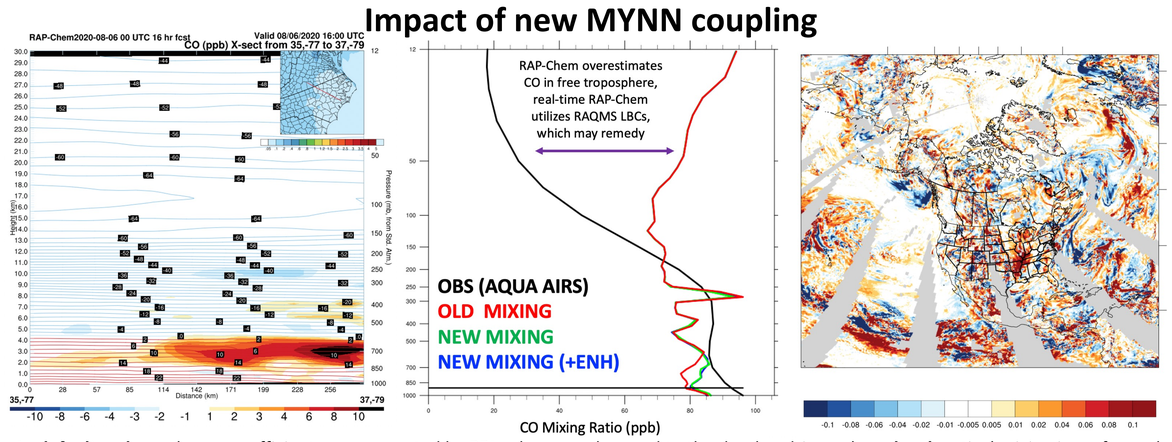
Interestingly, minimal temperature decreases during following days, indicating more buildup at the surface compared to the column

Sept Stats	*noFDB*		*w/ FDB*
Mean Bias:	1.6°C	vs.	1.4°C
RMSE:	3.9°C	vs.	3.6°C
Correlation:	0.70	vs.	0.74

Aerosol impacts on ozone forecast

The **inclusion of the direct aerosol effect** on photolysis also significantly reduces O_3 production (with likely small impacts from temperature reductions) and brings the model much closer to **observations**

Impact of new MYNN coupling



- **In default code,** exchange coefficients are computed by PBL scheme and passed to the dry dep driver where ***local*** vertical mixing is performed with dry deposition. ***NEW*** code passes deposition velocities (computed in /chem) to PBL scheme (in /phys) and performs non-local mixing alongside dry deposition
- In general, the impact of the new code is to reduce surface concentrations and increase concentrations aloft
- Initial comparisons between old and new code demonstrate improved correlations with AQUA AIRS CO profiles.