Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM) for Improving Air Quality Modeling

What is CRACMM?

EPA scientists are leading a collaboration with researchers in the scientific community to develop the Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM; pronounced CRACK-um). This new chemical mechanism is being designed to predict multiple air quality endpoints, including ozone (O_3), particulate matter (PM), chemical components of PM such as secondary organic aerosol (SOA), and toxics like formaldehyde. CRACMM will also be able to incorporate scientific advancements on topics such as autoxidation, aromatic chemistry, oxygenated hydrocarbons, organic nitrates, and halogens.

Why is CRACMM Being Developed?

EPA strives to ensure that the air quality models it uses – such as the Community Multiscale Air Quality (CMAQ) model – incorporate current state-of-the-science approaches. In air quality modeling, chemical mechanisms are used to represent atmospheric chemical reactions. How accurately the model makes predictions depends in part on how well those chemical mechanisms approximate the actual chemical processes in the atmosphere. Chemical mechanisms are updated to include newly discovered reactions, SOA yields, chemical properties and other new advances as the state-of-science develops.

For example, reactive organic carbon (ROC) is one important focus of CRACMM's development. ROC emissions have evolved over time as air quality regulations have been enacted. In the past, motor vehicles were the dominant emitters of ROC. Today, the relative dominance of ROC emissions has shifted toward sources like volatile chemical products (e.g., paints, solvents, adhesives) and wood burning. EPA is improving methods for chemically speciating the ROC emissions in EPA's National Emissions Inventory. Additionally, EPA researchers are examining reaction pathways for ROC to determine the best approaches to include in CRACMM.

Research is also underway to incorporate new scientific knowledge into CRACMM related to simulating different phases of chemicals (e.g., gas, aerosol). For example, most air quality models use chemical mechanisms that represent gas-phase chemistry only and rely on other development efforts to predict aerosols. CRACMM will instead specify the chemistry leading to both gas and particle endpoints. This approach will help models more closely replicate the photochemical processes that occur in the atmosphere.

How is CRACMM Being Built?

EPA and collaborators are building CRACMM on an existing chemical mechanism — version 2 of the Regional Atmospheric Chemical Mechanism (RACM2). RACM2 was chosen because it facilitates treatment of both ozone and SOA; is transparent in its emissions mapping; can be easily modified; and already has partners available who can contribute developments. EPA is adopting a community approach in developing CRACMM and will be seeking contributions from

the modeling community. By releasing an early version of the base research model, EPA will make it easier for potential collaborators to contribute to the mechanism development.

How Will CRACMM be Used in the Near-Term?

CRACMM will be incorporated into CMAQ and shared with partners who can incorporate it into other air quality and chemical transport models. In the 2021-2022 timeframe, EPA researchers anticipate using CRACMM as part of CMAQ modeling to address research questions and to continually test CRACMM performance.

How Will Users Obtain Model Inputs (Emissions and Boundary Conditions) for use with CRACMM?

Along with the 2022 CMAQ release, EPA plans to release a tool repository and inputs to support the creation of emissions, initial conditions, and boundary conditions for CRACMM. This will include inputs for the speciation of emissions. When simple mappings between mechanisms are appropriate, those will be included as well.

CRACMM Tentative Timeline

- Through the remainder of 2021 and 2022, the CRACMM team will be focused on developing, testing, evaluating, and documenting CRACMM. They will also update other CMAQ tools for processing model inputs needed for CRACMM. Toward the end of 2022, the team anticipates releasing CRACMM as a research option in CMAQv6, however CB6r5 is expected to remain the default chemical mechanism.
- In later years (i.e., 2023 through 2025), the CRACMM team anticipates continuing to focus on developing, testing, evaluating, and documenting for the contiguous U.S. and specifically evaluating CRACMM with field research campaigns. The team also plans to release semi- and intermediate volatile organic compound emission profiles for mobile and other emission sources compatible with the CRACMM system. Additionally, the team plans to compare the analyses of the CB6r5 and CRACMM chemical mechanisms, including analyzing sensitivity to changes in emissions.
- The CRACMM team anticipates that by the time of the expected 2025 CMAQ release, CRACMM will have been fully developed, tested, evaluated, and documented to support its use as the default mechanism in CMAQ. The CB6r5 and SAPRC chemical mechanisms will remain available for use with CMAQ, however updates to these mechanisms are not expected to be led by EPA researchers past 2022.
- Throughout the current and future years of development, the CRACMM team will continue communicating about their progress through scientific conferences, modeling community meetings, and manuscript submissions to peer-reviewed scientific journals.

Additional Resources

- CMAQ: The Community Multiscale Air Quality Modeling System https://www.epa.gov/cmaq
- CMAQ Chemical Process Overview https://www.epa.gov/cmaq/chemical-process-overview

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