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

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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 including that with diameters <2.5 µm, $PM_{2.5}$), chemical components of PM such as secondary organic aerosol (SOA), and toxic air pollutants like formaldehyde. CRACMM incorporates scientific advancements on topics such as aromatic chemistry, oxygenated hydrocarbons, organic nitrates, halogens, and autoxidation of hydrocarbons (see Table 1 from Pye et al., 2023). The first version of CRACMM was part of the 2022 CMAQv5.4 release and additional updates are planned in 2024 and 2026.

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 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 represent the 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. Over time, ROC emissions have shifted toward sources like volatile chemical products (e.g., paints, solvents, adhesives), wood burning (e.g., wildland fires and residential wood burning), and biogenic sources. EPA is improving methods for chemically speciating the ROC emissions in EPA's National Emissions Inventory (Murphy et al., 2023; Seltzer et al. 2023). 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 both the gas- and aerosol-phase composition. For example, most air quality models use chemical mechanisms that represent gas-phase chemistry only and rely on separate algorithms to predict aerosols. CRACMM specifies the chemistry leading to both gas and particle endpoints such as ozone and $PM_{2.5}$. This approach will help models more closely replicate the photochemical processes that occur in the atmosphere.

How is CRACMM Being Built?

EPA has adopted a community approach in developing CRACMM. The first version of CRACMM was based on an existing chemical mechanism — version 2 of the Regional Atmospheric Chemical Mechanism (RACM2, Goliff et al., 2013). RACM2 facilitates treatment of both ozone and SOA; is transparent in its emissions mapping; can be easily modified; and has partners available who can contribute developments. By releasing CRACMM in CMAQv5.4 and using open software development principles, EPA has made it easier for collaborators to contribute to the mechanism development. In CRACMM version 1 (Pye et al., 2023), NOAA's Chemical Sciences Laboratory contributed to the development of alkane, furan, and propylene glycol chemistry. The University of Colorado Boulder contributed to aromatic chemistry. The University of Texas El Paso contributed rate constant and photolysis reaction updates, and Columbia University developed isoprene chemistry (Wiser et al., 2023).

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

Tools and data are available to develop model inputs for CMAQ-CRACMM. CMAQv5.4 and its utilities allow users to create initial and boundary conditions for CRACMM. CRACMM provides tools to automate the mapping of specific emitted compounds to the CRACMM chemical mechanism species (see Pye et al., 2023). Emissions tools such as S2Stool and SMOKE have been developed or expanded to ensure CRACMM compatibility. SMOKE-ready and CMAQ-ready inputs for CRACMM are also available to the public. For details on how to obtain this information, see https://github.com/USEPA/CRACMM.

When will CRACMM become available?

- The first version of CRACMM was publicly released in 2022 as a research option in CMAQv5.4. This version of CRACMM has now been tested and documented in the peer-reviewed literature (Pye et al., 2023; Place et al., 2023; Wiser et al., 2023; Seltzer et al., 2023). Our model evaluation indicates compared to CMAQv5.4 with the Carbon Bond chemical mechanism, summer organic carbon $PM_{2.5}$ is considerably improved, while ozone concentrations and their sensitivity to broad emission changes are similar.
- The CMAQ team is planning a mid-cycle release in 2024 and a major release in 2026 that will include updates to CRACMM. The CRACMM team anticipates continuing to develop, test, evaluate, and document predictions for the contiguous U.S. and northern hemisphere. In addition to routine network data, CRACMM will be evaluated with specialized measurements from field research campaigns and used to understand the sensitivity of predictions to emissions.
- The CMAQv5.4 Carbon Bond and SAPRC mechanisms will be available as options in the 2024 and 2026 CMAQ releases. EPA is not planning to develop further science improvements beyond the CMAQv5.4 version of these mechanisms.
- If the community has a particular interest in updates to a chemical system or approaches to chemical mechanism representation, they can work with the CRACMM team to determine how to make their updates available in CRACMM so the community receives the broadest scientific benefit. Please reach out to the CRACMM project lead investigator who will

coordinate how to proceed with updates. For situations where this is not feasible, a CMAQ community contribution can be made (see the CMAQ Developers Guide).

- Throughout the current and future years of development, the CRACMM team will continue communicating updates 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

Publications

- Goliff, W. S., Stockwell, W. R., and Lawson, C. V.: The regional atmospheric chemistry mechanism, version 2, Atmos. Environ., 68, 174-185, https://doi.org/10.1016/j.atmosenv.2012.11.038, 2013.
- Place, B. K., Hutzell, W. T., Appel, K. W., Farrell, S., Valin, L., Murphy, B. N., Seltzer, K. M., Sarwar, G., Allen, C., Piletic, I. R., D'Ambro, E. L., Saunders, E., Simon, H., Torres-Vasquez, A., Pleim, J., Schwantes, R. H., Coggon, M. M., Xu, L., Stockwell, W. R., and Pye, H. O. T.: Sensitivity of northeastern US surface ozone predictions to the representation of atmospheric chemistry in the Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMMv1.0), Atmos. Chem. Phys., 23, 9173–9190, https://doi.org/10.5194/acp-23-9173-2023, 2023.
- Pye, H. O. T., Place, B. K., Murphy, B. N., Seltzer, K. M., D'Ambro, E. L., Allen, C., Piletic, I. R., Farrell, S., Schwantes, R. H., Coggon, M. M., Saunders, E., Xu, L., Sarwar, G., Hutzell, W. T., Foley, K. M., Pouliot, G., Bash, J., and Stockwell, W. R.: Linking gas, particulate, and toxic endpoints to air emissions in the Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM), Atmos. Chem. Phys., 23, 5043–5099, https://doi.org/10.5194/acp-23-5043-2023, 2023.
- Murphy, B. N., Sonntag, D., Seltzer, K. M., Pye, H. O. T., Allen, C., Murray, E., Toro, C., Gentner, D. R., Huang, C., Jathar, S. H., Li, L., May, A. A., and Robinson, A. L.: Reactive Organic Carbon Air Emissions from Mobile Sources in the United States, EGUsphere, 2023, 1-24, https://doi.org/10.5194/egusphere-2023-855, 2023.
- Seltzer, K. M., Rao, V., Pye, H. O. T., Murphy, B. N., Place, B. K., Khare, P., Gentner, D. R., Allen, C., Cooley, D., Mason, R., and Houyoux, M.: Anthropogenic secondary organic aerosol and ozone production from asphalt-related emissions, Environmental Science: Atmospheres, https://doi.org/10.1039/D3EA00066D, 2023.
- Wiser, F., Place, B. K., Sen, S., Pye, H. O. T., Yang, B., Westervelt, D. M., Henze, D. K., Fiore, A. M., and McNeill, V. F.: AMORE-Isoprene v1.0: a new reduced mechanism for gas-phase isoprene oxidation, Geosci. Model Dev., 16, 1801–1821, https://doi.org/10.5194/gmd-16-1801-2023, 2023.

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