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A computationally-efficient secondary organic aerosol module for three-dimensional air quality models

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Abstract. Accurately simulating secondary organic aerosols (SOA) in three-dimensional (3-D) air quality models is challenging due to the complexity of the physics and chemistry involved and the high computational demand required. A computationally-efficient yet accurate SOA module is necessary in 3-D applications for long-term simulations and real-time air quality forecasting. A coupled gas and aerosol box model (i.e., 0-D CMAQ-MADRID 2) is used to optimize relevant processes in order to develop such a SOA module. Solving the partitioning equations for condensable volatile organic compounds (VOCs) and calculating their activity coefficients in the multicomponent mixtures are identified to be the most computationally-expensive processes. The two processes can be speeded up by relaxing the error tolerance levels and reducing the maximum number of iterations of the numerical solver for the partitioning equations for organic species; conditionally activating organic-inorganic interactions; and parameterizing the calculation of activity coefficients for organic mixtures in the hydrophilic module. The optimal speed-up method can reduce the total CPU cost by up to a factor of 31.4 from benchmark under the rural conditions with 2 ppb isoprene and by factors of 10–71 under various test conditions with 2–10 ppb isoprene and >40% relative humidity while maintaining ±15% deviation. These speed-up methods are applicable to other SOA modules that are based on partitioning theories.

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