4.016 Development of a Global Atmospheric Chemistry Model for the Study of PAHs (EMAC-PAH) and Application.

Early Career Scientist

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Abstract:

The ECHAM/MESSy Atmospheric Chemistry (EMAC) model has today become a more favorable tool to simulate global tropospheric and stratospheric chemistry and climate. MESSy provides a framework for the interconnection of the base model (i.e., ECHAM5) and earth-system components, i.e., sub-models describing atmospheric composition, processes and its interaction with oceans, land and human activities. This framework makes the integral model very flexible for use in a wide variety of applications and its development has been continuous. In this work, we expanded the model to include simulations of the transport and fate of polycyclic aromatic hydrocarbons (PAHs) and other semi-volatile contaminants. These substances persist in environmental compartments and pose a health hazard and bio-accumulate along food chains. EMAC-PAH takes into account essential environmental processes including (1) gas-particle partitioning, (2) dry and wet depositions, (3) chemical and biotic degradations, and (4) volatilizations from ocean, land, vegetation, and snow. The gas-particle partitioning is based on a dual approach parameterization, assuming absorption into organic carbon (OC) and adsorption to black carbon (BC) aerosols. We selected four compounds for study, spanning a wide range of volatility, i.e., phenanthrene (PHE), anthracene (ANT), fluoranthene (FLT), and benzo[a]pyrene (BaP). Simulations were carried out to study the significance of homogeneous and heterogeneous oxidations. Observation data from multiple land monitoring networks, including the Arctic, and two ship measurements during 2007-2009 were employed to evaluate the model performance.