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Supplement of

Toward a learnable Artificial Intelligence Model for Aerosol Chemistry and Interactions (AIMACI) based on the Multi-Head Self-Attention algorithm

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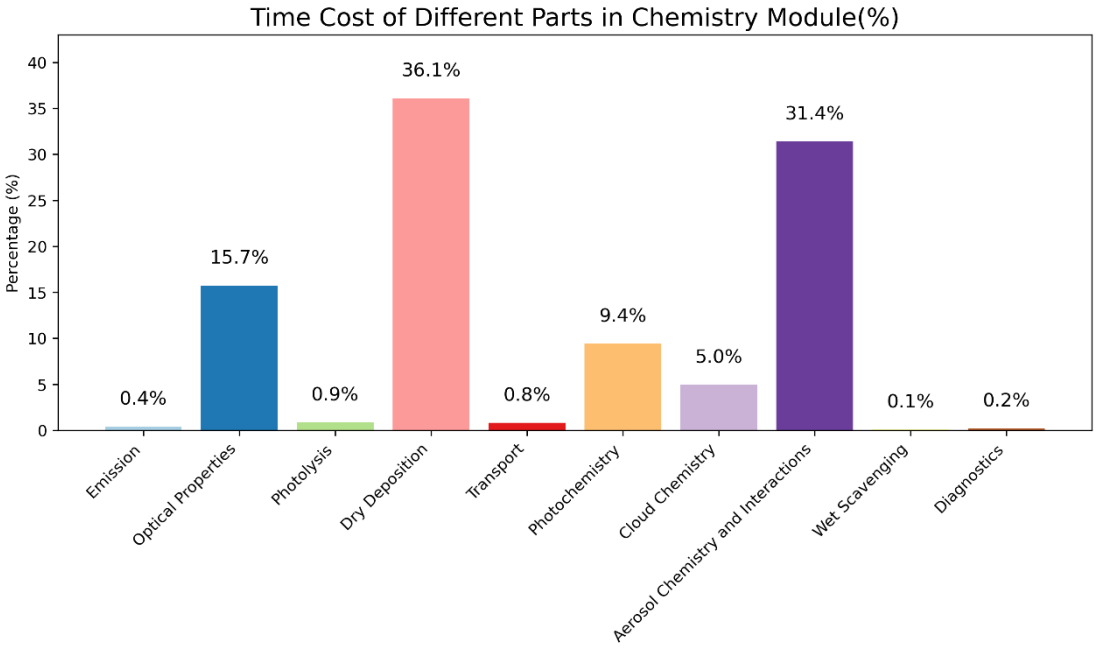

Figure S1: Proportion of computational time for different parts of the chemistry module in this study. The photochemistry is modeled using the CBM-Z (Carbon Bond Mechanism Version Z) scheme, which does not account for gas species related to complex SOA, while aerosol chemistry and interactions are simulated using the Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) scheme, which primarily focuses on inorganic aerosol species and utilizes a 4-bin configuration.

(a) Pseudo-code for original chemistry model

```
subroutine chem_driver
    defining interfaces
    defining variablers
    initializing data
    for each tile
        call emissions_driver
        call optical_driver
        call photolysis_driver
        call dry_dep_driver
        call grelldrvct
        call mechanism_driver
        call cloudchem_driver
        call aerosols_driver
            call mapaer_tofrom_host
            call mosaic_dynamic_solver
            call move_sections
            call mosaic_newnuc_1clm
            call mosaic_coag_1clm
            call mapaer_tofrom_host
        call wetscav_driver
        call budget_calc
    end for
end subroutine chem_driver
```

(b) Pseudo-code for AI-mixed chemistry model

```
subroutine chem_driver
    defining interfaces
    defining variablers
    initializing data
    for each tile
        call emissions_driver
        call optical_driver
        call photolysis_driver
        call dry_dep_driver
        call grelldrvct
        call mechanism_driver
        call cloudchem_driver
        call AIMACI
        call wetscav_driver
        call budget_calc
    end for
end subroutine chem_driver
```

Figure S2: Schematic diagram of the specific components replaced by the AIMACI scheme in WRF-Chem. (a) The pseudo code for original chemistry model in WRF-Chem. The part surrounded by the blue dotted box is the key subroutine inside aerosols_driver. (b) The pseudo code for AI-mixed chemistry model in WRF-Chem. The AIMACI scheme enables end-to-end simulation of full aerosol chemistry and interactions processes, including chemical reactions, phase equilibrium, gas-particle partitioning, particle size growth, coagulation, and nucleation. Note that in our study, the chosen MOSAIC scheme features four discrete size bins and primarily focuses on processes related to inorganic aerosols. It also considers the impact of marine biogenic sources of dimethyl sulfide on atmospheric aerosols and some aqueous reactions. However, secondary organic aerosols and complex heterogeneous chemical processes are not included in the chosen MOSAIC scheme. These aspects will be considered for future development.

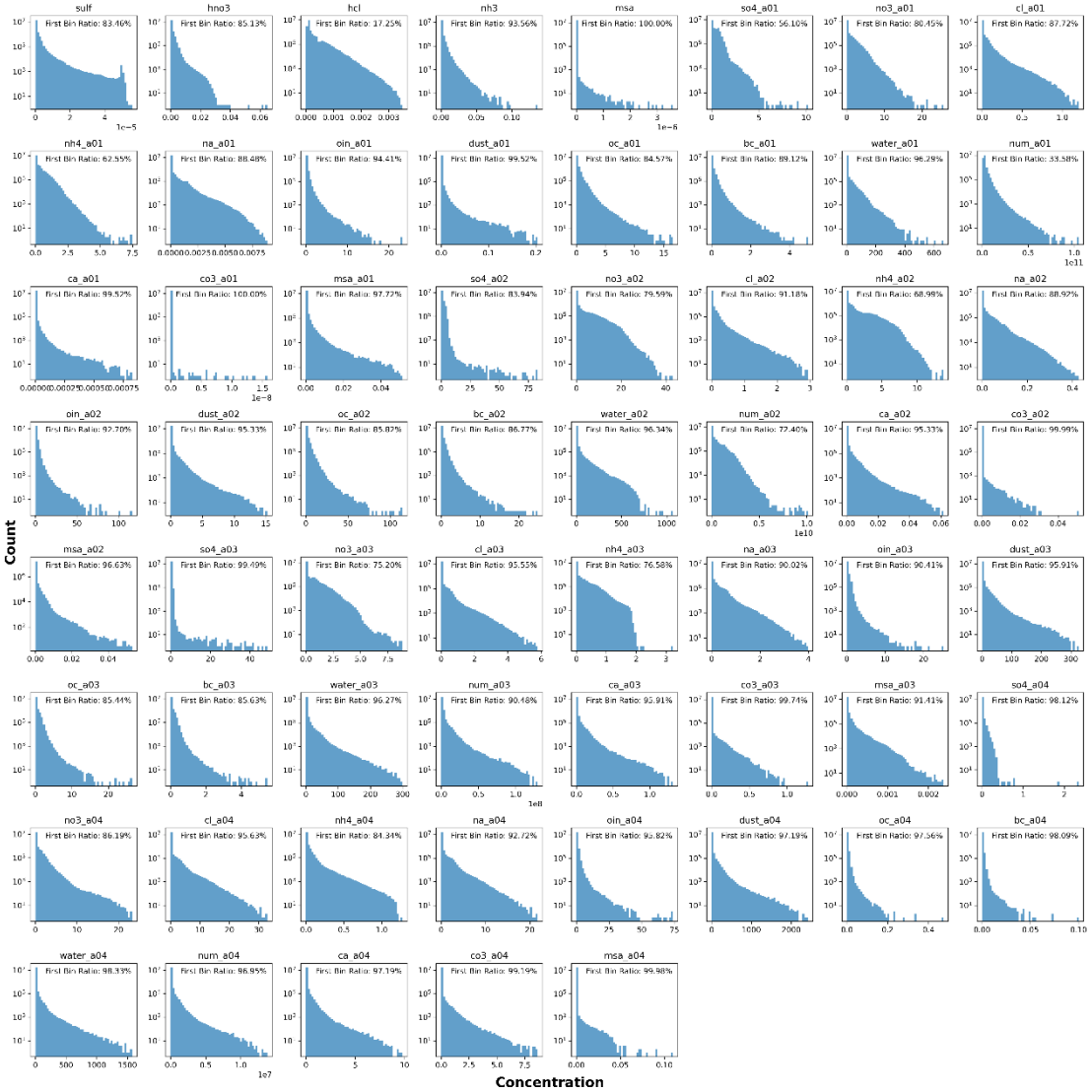

Figure S3: Frequency distribution of concentrations for all output targets in the test dataset.

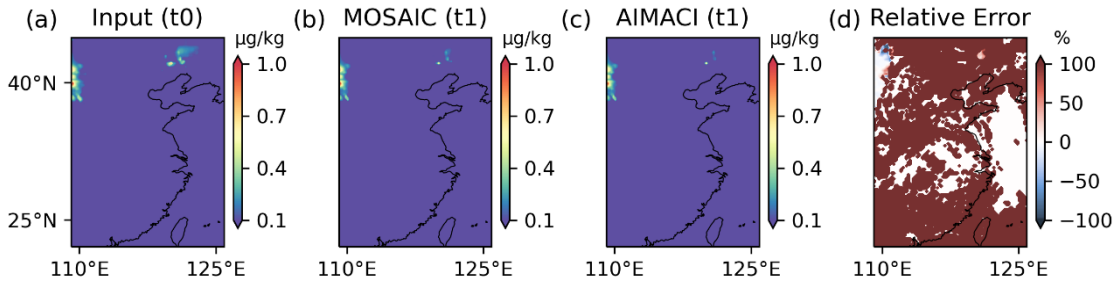

Figure S4: The spatial distribution of carbonate surface concentrations in the 0.625–2.5 μm particle size range (CO_3_a03) simulated by both MOSAIC and AIMACI scheme at 2019-03-19-16:00:00(UTC).