Supplementary Information for

# Incorporating An Advanced Aerosol Activation Parameterization into WRF-CAM5: Model Evaluation and Parameterization Intercomparison

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**Introduction**

This supplementary file describes (1) WRF-CAM5 testing of the two activation parameterizations, (2) the emissions of chemical species before and after adjustment in 2005 and 2010 used for the baseline simulations, and (3) additional results that supplement results discussed in the main text.

**Text S1.**

**Description of WRF-CAM5 testing of the two activation parameterizations**

As mentioned in Section 2.2, there are three major differences between treatments in AR-G00 and FN05 parameterizations. First, AR-G00 uses a constant temperature (i.e., 273 K) in calculating surface tension and Kelvin effect in AR-G00, whereas FN05 accounts for their temperature dependence. Second, AR-G00 assumes 1.0 for the condensation coefficient of water vapor, and neglects gas kinetic effect, whereas FN05 assumes a value of 0.06 and treats the gas

kinetic effects by using an average value of water vapor diffusivity over an appropriate size range. Third, AR-G00 uses an empirical relationship to approximate $S_{max}$, whereas FN05 uses numerical iterations to solve $S_{max}$.

To examine the relative importance of the three major factors to the differences in the simulated aerosol activation fractions by the two parameterizations, a set of three-hour test simulations with 180-second time step using WRF-CAM5 with the two parameterizations are performed. The test period is 00:00-03:00 (UTC) June 25th, 2005 and the test domain is East Asia. Output frequency is every time step. Four simulations have been performed. Table S1 summarizes their basic configurations. AR-G00DEF and FN05DEF are simulations with default AR-G00 and FN05 parameterization. ARG00MOD uses the same method with the FN05 parameterization in the calculation of surface tension and Kelvin effect with the dependence on temperature. FN05MOD uses the same value of the condensation coefficient of water vapor (a value of 1.0) in the calculation, same as that used in AR-G00 parameterization.

Results from 6-minute output (the 2nd time step) and 3-hour (the 60th time step) are extracted and analyzed. The 2nd time step outputs from different simulations have very small differences since the feedbacks have not been accumulated yet (note that the first step results are not used because aerosol number concentrations are very low at the very beginning and everything is just initialized). The 60th time step results are expected to be affected by feedbacks. The grid point data of these simulations are extracted and analyzed. Only the data from the 2nd time step is extracted, and the grid cells that did not call the aerosol activation module are neglected. The number fractions of activated aerosol for coarse mode are not shown because in all simulations they are equal or closed to one. Due to the decrease of $S_c$ from ARG00DEF to ARG00MOD, $S_{max}$ slightly decreases leading to more particle growth and water absorption.

Between ARG00MOD and ARG00DEF, major differences lie in the treatment of the temperature-dependence of surface tension and Kelvin. For the 2nd time step, comparing to ARG00DEF, ARG00MOD gives domain-average of 10% and 12% higher number fraction of activated aerosol for accumulation and Aitken modes, respectively. Between FN05MOD and ARG00MOD, major differences lie in the method of solving $S_{max}$. Comparing ARG00MOD, FN05MOD gives 10-20% higher $S_{max}$ over land and 50-100% higher $S_{max}$ over ocean, leading to a significant increase from ARG00MOD to FN05MOD in predicting number fractions of activated aerosols in accumulation and Aitken modes by 15% and 19% on average, respectively. The difference between FN05DEF and FN05MOD is in the value of water vapor condensation coefficient. Comparing to FN05MOD, FN05DEF gives constantly 30% higher $S_{max}$ than FN05MOD, leading to a 15% increase in predicting number fraction of activated aerosols in accumulation and Aitken mode. For the 2nd time step, comparing to ARG00DEF, FN05DEF gives ~50% higher CCN, with ~20% due to the different water vapor condensation coefficients used, ~20% due to the different methods in solving max supersaturation, and another ~10% due to the calculation of Kelvin effects. For the 60th time step, the differences in activation fractions due to the calculation of Kelvin effects, different water vapor condensation coefficients, and the different methods in solving max supersaturation increase to 15.3%, 23.0%, and 69.9%, respectively, which reflect the feedback effects that are accumulated since the 2nd time step of the calculation.

**Text S2.**

**Emissions of chemical species before and after adjustment in 2005 and 2010**

Table S2 compares total emissions over all emission layers before and after adjustment for 2005 and 2010 used in the baseline simulations. As shown, the adjusted emissions of major species including CO, $SO_2$, $NH_3$, NO, $NO_2$, $PM_{10}$, sulfate, elemental carbon, organic carbon, and other unknown fine PM are higher than those un-adjusted emissions by 1.7-327% in 2005 and by 3.7-318.6% in 2010.

Table S1. Testing simulations to examine factors contributing to differences between WRF-CAM5 simulations with AR-G00 and

FN05

| Simulation ID | Parameterization | Modification | Notes |
| --- | --- | --- | --- |
| ARG00DEF | AR-G00 | Default | The calculation of surface tension and Kelvin effect uses a constant temperature of 273K in every call. |
| ARG00MOD | AR-G00 | Surface tension and Kelvin effect are temperature-dependent | The calculation of surface tension and Kelvin effect are set to be the same as that of FN05. |
| FN05DEF | FN05 | Default | Water vapor condensation coefficient of 0.06 is used |
| FN05MOD | FN05 | Water vapor condensation coefficient changed to 1.0 | Water vapor condensation coefficient is set to be the same as that in AR-G00 |

Table S2. Total emissions before and after adjustment for 2005 and 2010

| Species | 2005 | | | 2010 | | |
|---------|------|------|------|------|------|------|
| | Before adjustment | After adjustment | % change | Before adjustment | After adjustment | % change |
| E_CO | 437722 | 531181 | 21.4 | 405620 | 496261 | 22.3 |
| E_SO2 | 31750 | 31750 | 15.2 | 26083 | 30337 | 16.3 |
| E_NH3 | 55438 | 74228 | 33.9 | 40769 | 54673 | 34.1 |
| E_NO | 26552 | 37112 | 39.8 | 33299 | 49953 | 50.0 |
| E_NO2 | 2950 | 4124 | 39.8 | 3700 | 5550 | 50.0 |
| E_PM10 | 114 | 157 | 37.9 | 77 | 110 | 42.4 |
| E_SO4J | 54541 | 74602 | 36.8 | 35309 | 50653 | 43.5 |
| E_ECJ | 119465 | 178604 | 49.5 | 109063 | 164269 | 50.6 |
| E_ORGJ | 320170 | 1367082 | 327.0 | 279791 | 1171281 | 318.6 |
| E_PM25J | 390634 | 449843 | 1.7 | 385131 | 399374 | 3.7 |

The unit of the emissions is mol $km^{-2}$ $hr^{-1}$ for all gaseous species and $PM_{10}$, and g $km^{-2}$ $yr^{-1}$ for other species (i.e., ECJ, ORGJ, PM25J, and SO4J).