

Consider a first order chemical reaction in which
Chemical 1 is converted to Chemical 2



$$\text{Rate} = k C_1$$

$$\frac{dC_1}{dt} = -kC_1$$

$$C_1(t) = C_1(0)e^{-kt}$$

$$C_2(t) = C_1(0) - C_1(t)$$

$$C_2(t) = C_1(0) (1 - e^{-kt})$$

$$M_2(t) = M_1(0) (1 - e^{-kt})$$

For values of chemical rxn time constant $\beta = kt < 0.01$, $M_2 \approx M_1(0)kt$

If the molecular weight (W_2) of C_2 is different from the molecular weight (W_1) of C_1 , then the mass of C_2 is increased by the ratio of molecular weights, i.e.,

$$M_2(t) = M_1(0) (1 - e^{-kt}) (W_2/W_1)$$

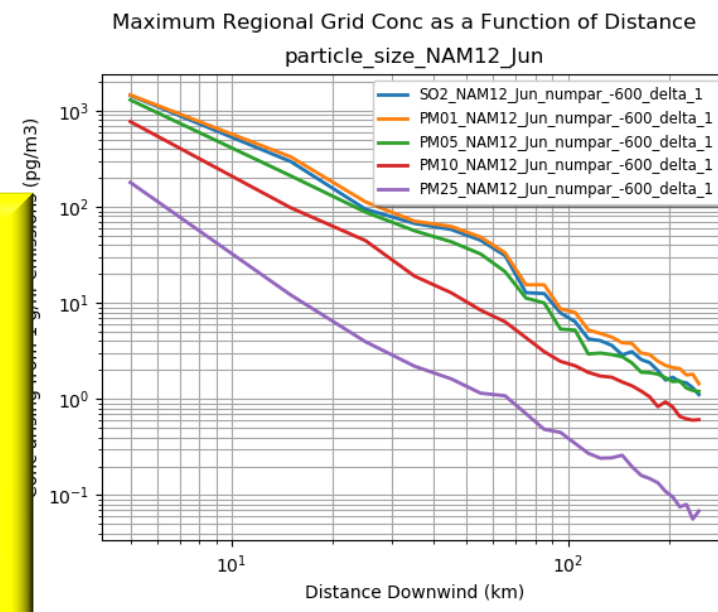
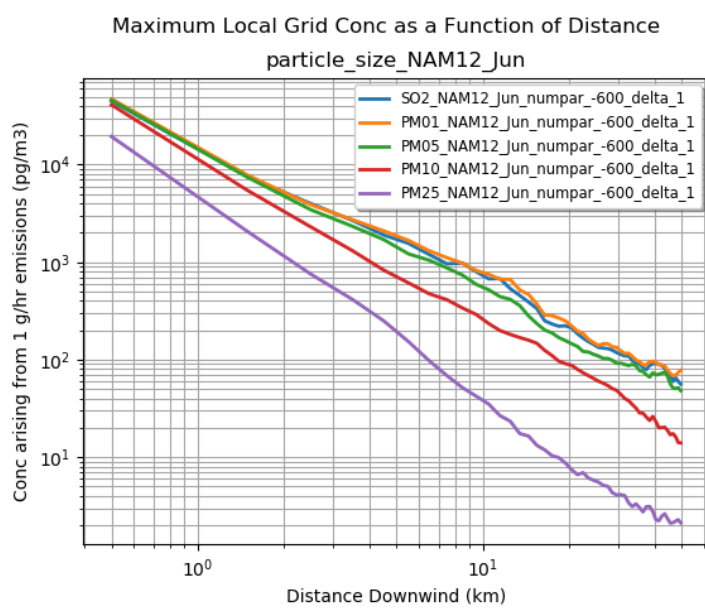


Molecular weight of $SO_2 = 64$

Molecular weight of $SO_4^{-2} = 96$

Ratio = 1.5

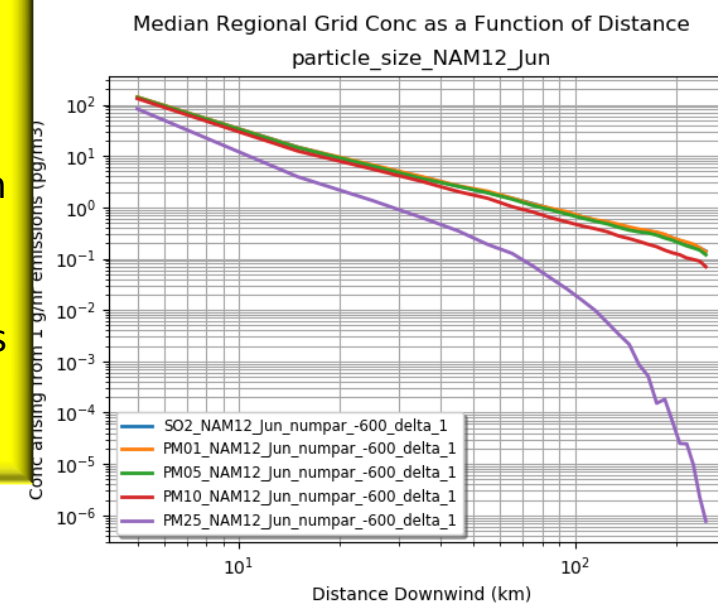
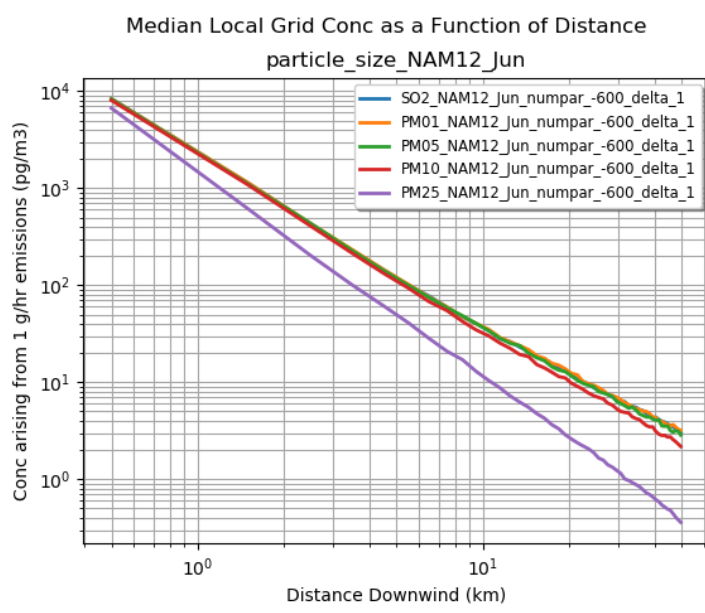
For every amount of mass that SO_2 is depleted by the reaction, the mass of SO_4^{-2} increases by 1.5 x that amount of mass (the conversion adds two extra oxygen atoms to the molecule)



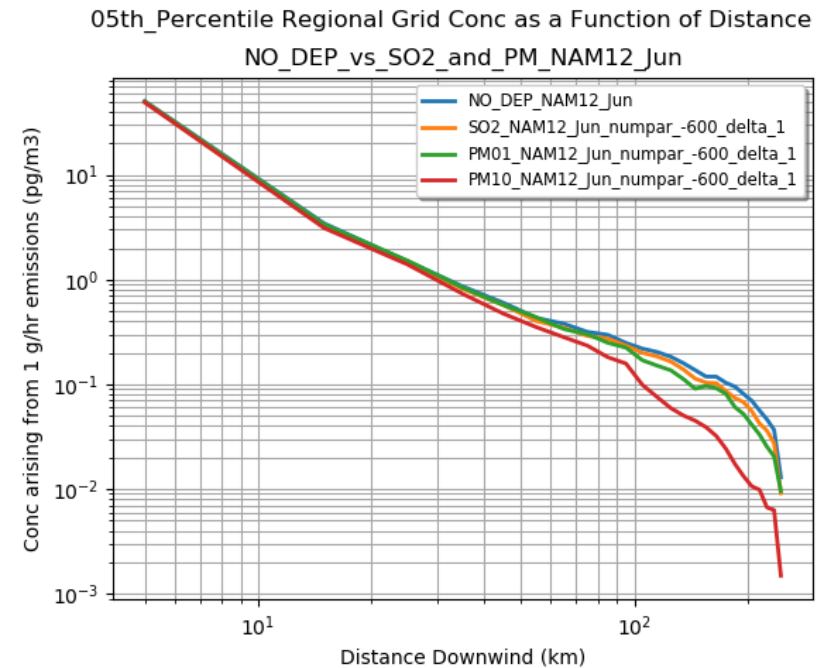
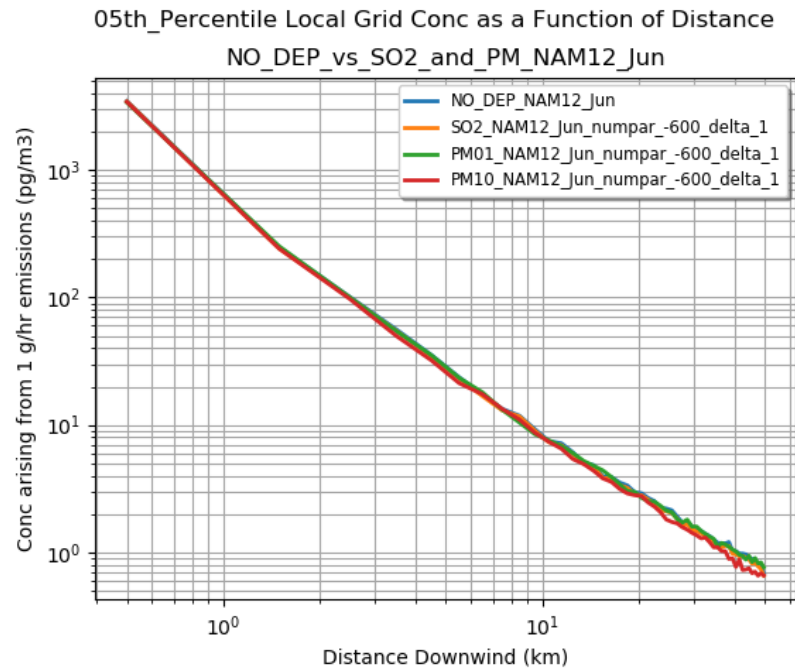
Not a very dramatic difference between gas-phase SO₂, and 1 and 5 μm particles

If pollutant partitions to atmospheric particles, most would be associated with particles less than 5 μm

Bigger differences seen with 10 and 25 μm particles

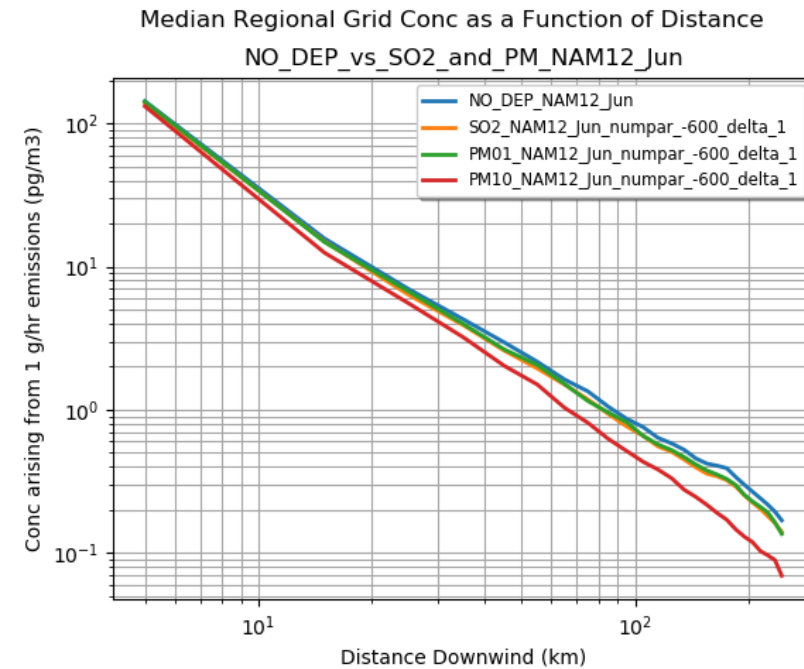
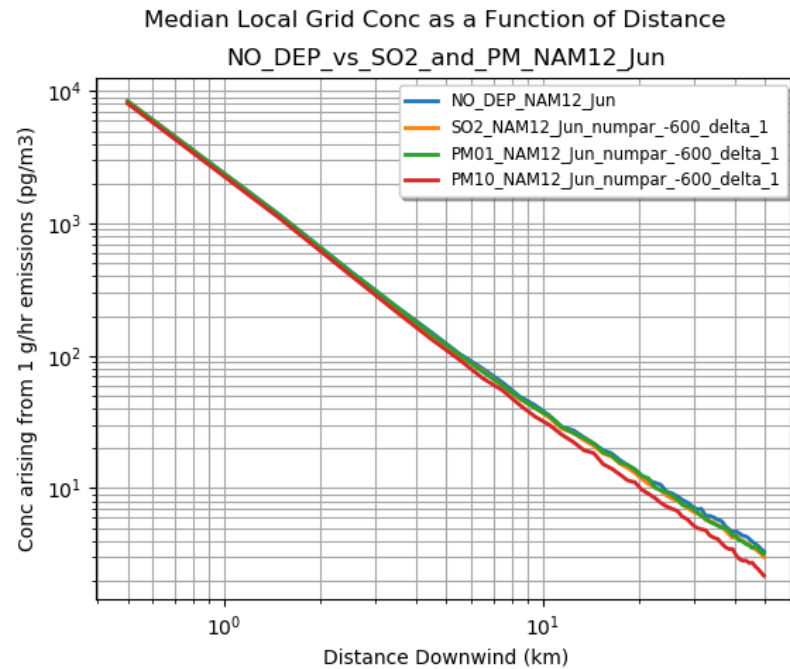


Compare simulation with no deposition with simulation of SO₂, PM₀₁ and PM₁₀ with default deposition parameters



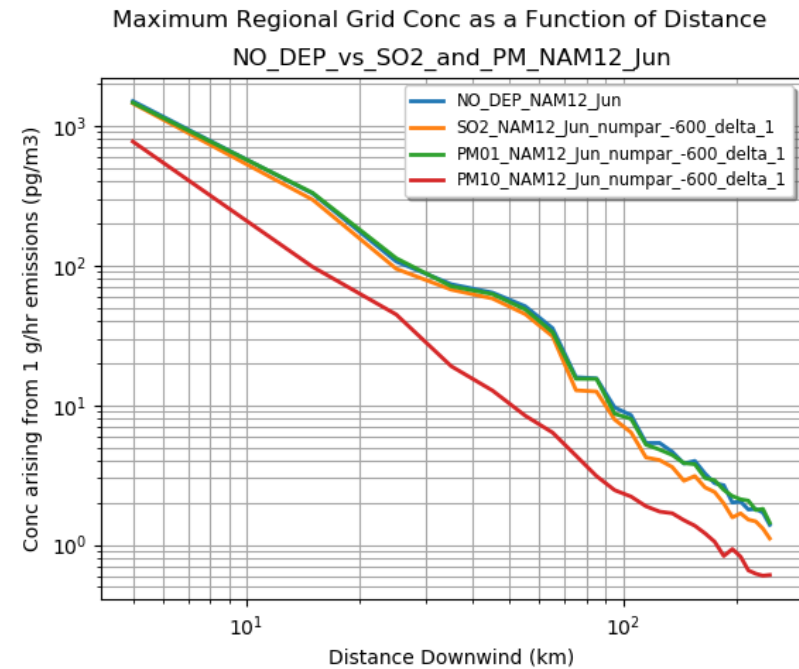
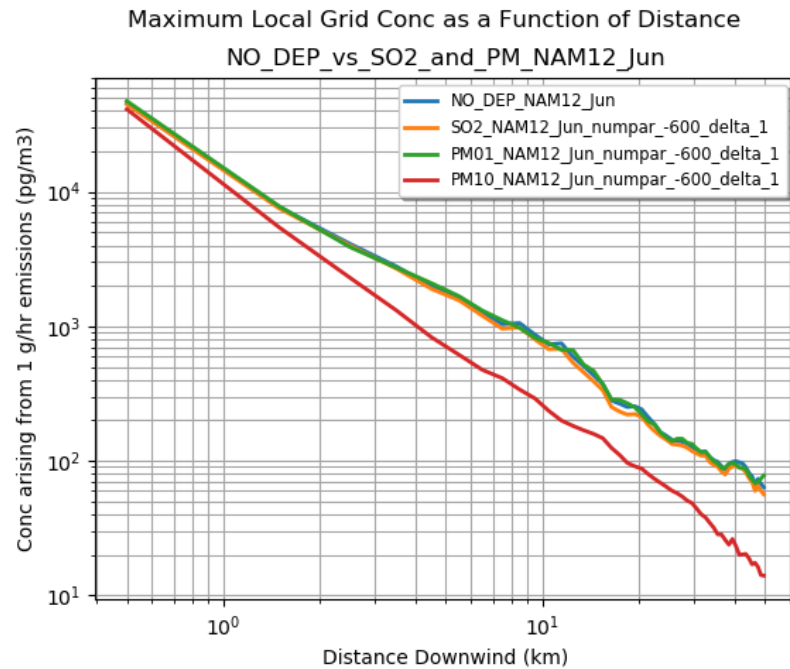
For 5th percentile, where one might expect to see the consequences of deposition (e.g., when it is raining), little difference except for large distances with large particles (10 μm)

Compare simulation with no deposition with simulation of SO₂, PM₀₁ and PM₁₀ with default deposition parameters



For median concentrations, little difference except for large particles (10 μm)

Compare simulation with no deposition with simulation of SO₂, PM₀₁ and PM₁₀ with default deposition parameters



For maximum concentrations, little difference except for large particles (10 μm)

Example of overall impact of wet/dry deposition (for SO₂)

Statistical Distribution of Hourly Concentration Values

local_grid_9.5_km

