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The capabilities of the adjoint of GEOS-Chem model to support HEMCO emission inventories and MERRA-2 meteorological data

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Supplemental Information

Inventory	Area	Resolution	Frequency	Period	Sector		Data source	Scaling factor	The time range of the factor
CEDS	Global	0.5x0.5	monthly	1750-2019	1. Agriculture 2. Energy 3. Industry 4. On-Road Transportation 5. Non-Road/Off-Road Transportation 6. Residential Combustion	7. Commercial Combustion 8. Other Combustion 9. Solvent production and application 10. Waste 11. International Shipping	McDuffie,et al.(2020)	Diurnal scale factors	24 hours
MIX	Asia	0.25x0.25	monthly	2008-2010	1.Power plants 2.Industry	3.Residential 4.Transportation	Li, M.,et al(2017)	AnnualScalar.geos.1x1.nc	1985-2010
								Diurnal scale factors	24 hours
NEI2011	North America	0.1x0.1	monthly	2011	1. Surface inventory 2. other point sources 3. non-EGU industrial stacks 4. ships	5. electric generating units (EGUs) 6. peaking electric generating units (EGUs) 7. oil and gas sector (new to NEI2011)	https://www.epa.gov/air-emissions-inventories/2011-national-emissions-inventory-nei-data	NEI11_CO_YRSCALE	2006-2013
								NEI99.dow.geos.1x1.nc	1999/1~12
DICE_AFRICA	Africa	0.1x0.1	yearly	2016	1.Household fuelwood use 2.Commercial fuelwood use 3.Crop residue for energy 4.Charcoal use 5.Charcoal production 6.Kerosene use	7.Cars (gasoline and diesel use) 8.Motorcycles (gasoline and diesel use) 9.Household fuelwood use 10.Household generator use 11.Natural gas flaring 12.Ad hoc oil refining	Marais,et al.	Diurnal scale factors	24 hours
EDGARV43	Global (Only applied in Africa here)	0.1x0.1	yearly	1970-2011	1.Power generation 2.Energy industry 3.Manufacturing industry 4.Road transport 5.Railways, pipelines, off-road transport 6.Energy for buidings (residential combustion)	7.Process emissions during production and application 8.Agriculture (excluding soil and agricultural burning) 9.Agricultural waste burning 10.Soil emissions 11.Waste solid and wastewater 12.Fossil Fuel Fires	Crippa, M.,et al	EDGAR_v43.Seasonal.1x1.nc	2010/1~12
								COPROD_FOSSIL=1.19	\
APEI	Canada	0.1x0.1	yearly	1989-2016	\		http://edgar.jrc.ec.europa.eu/overview.php?v=431	COPROD_FOSSIL=1.19	\
GFED4	Global	0.25x0.25	monthly	1997-2019	1.Total dry matter 2.Dry matter from temperate forests 3.Dry matter from peat 4.Dry matter from savanna	5.Dry matter from deforestation 6.Dry matter from boreal forest 7.Dry matter from agricultural waste	Randerson,et al.(2015)	GFED_emission_factors.txt	\
								Scaling_CO=1.05	\

Table S1. Updated emission inventories adopted in GC-Adjoint-HEMCO.

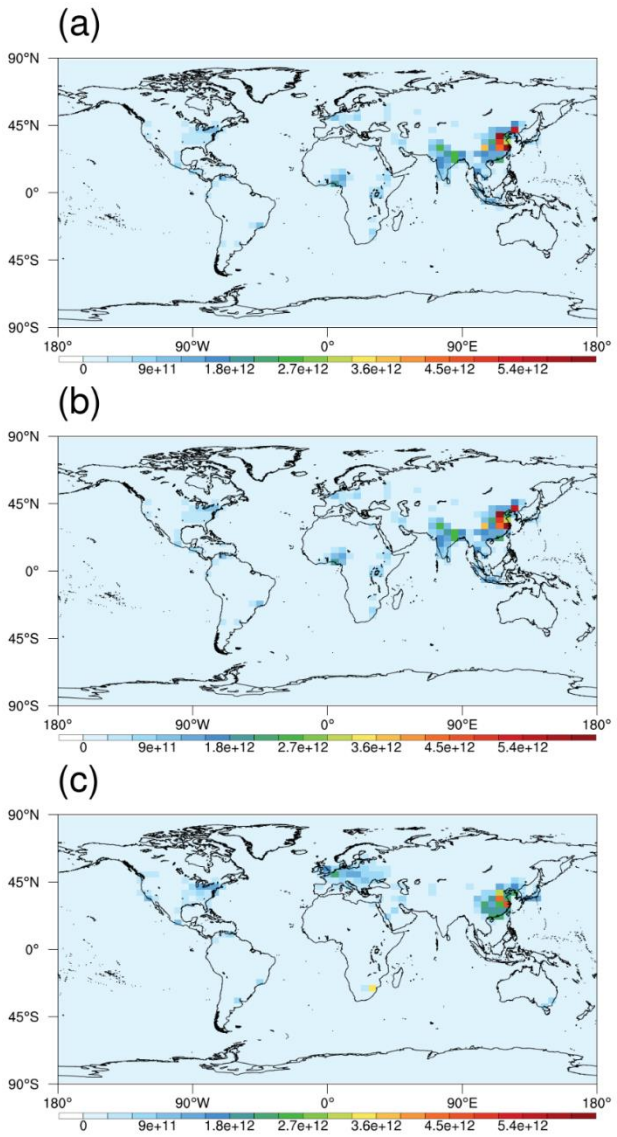

Fig. S1. CEDS CO emissions in 2015 from (a) GC-v12; (b) GC-Adjoint-HEMCO; and GEIA CO emissions in (c) GC-Adjoint-STD. The unit is molec/cm2/s.

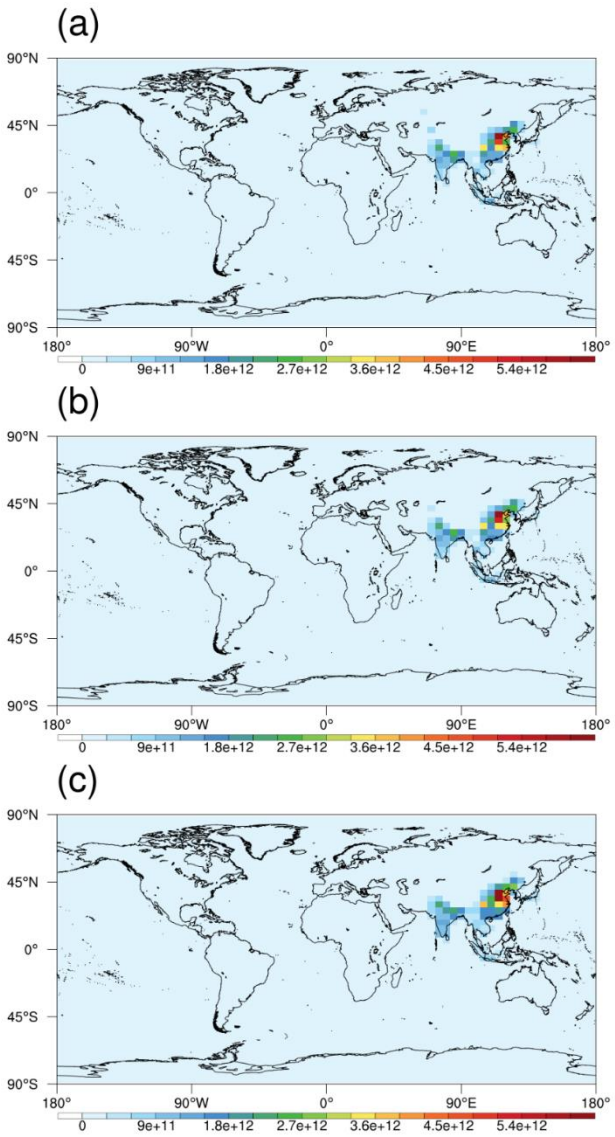

Fig. S2. MIX CO emissions in 2015 from (a) GC-v12; (b) GC-Adjoint-HEMCO; and INTEX-B CO emissions in (c) GC-Adjoint-STD. The unit is molec/cm2/s.

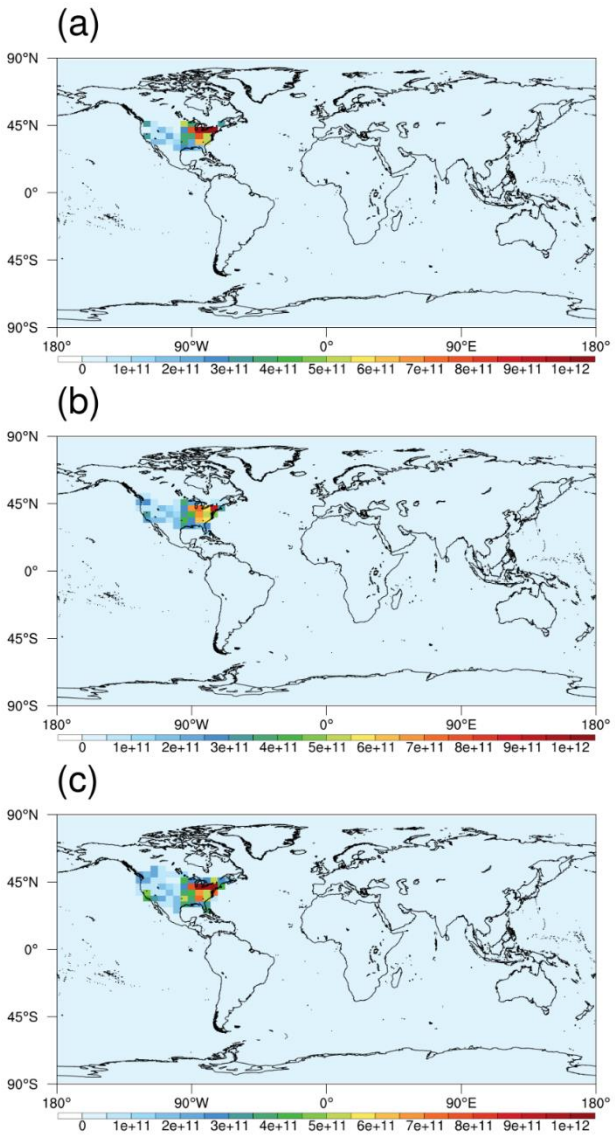

Fig. S3. NEI2011 CO emissions in 2015 from (a) GC-v12; (b) GC-Adjoint-HEMCO; and NEI2008 CO emissions in (c) GC-Adjoint-STD. The unit is molec/cm2/s.

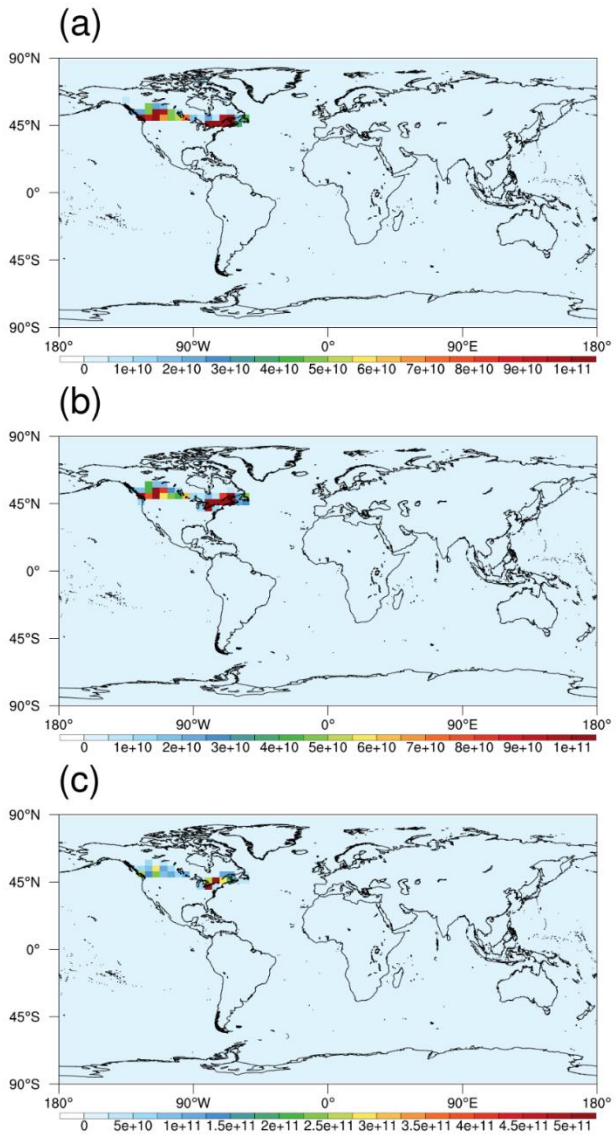

Fig. S4. APEI CO emissions in 2015 from (a) GC-v12; (b) GC-Adjoint-HEMCO; and CAC CO emissions in (c) GC-Adjoint-STD. The unit is molec/cm2/s.

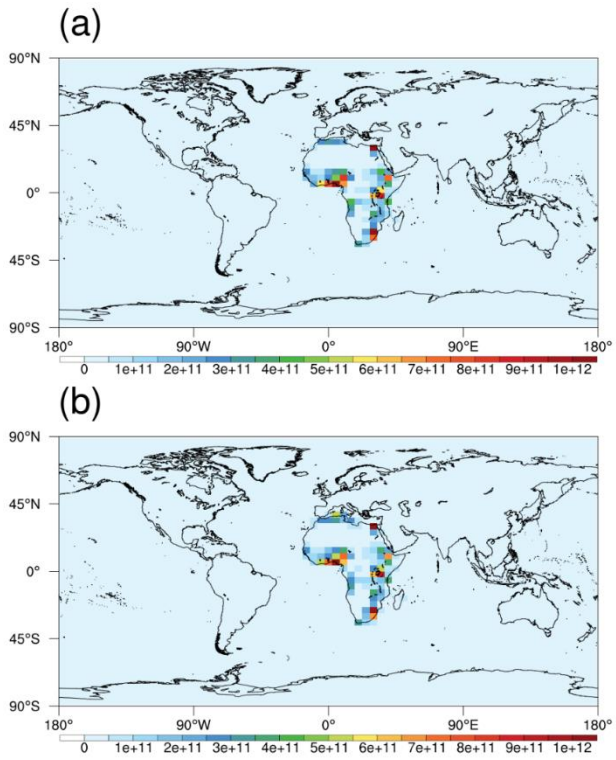

Fig. S5. DICE_AFRICA+AF_EDGAR CO emissions in 2015 from (a) GC-v12; (b) GC-Adjoint-HEMCO. The unit is molec/cm2/s.

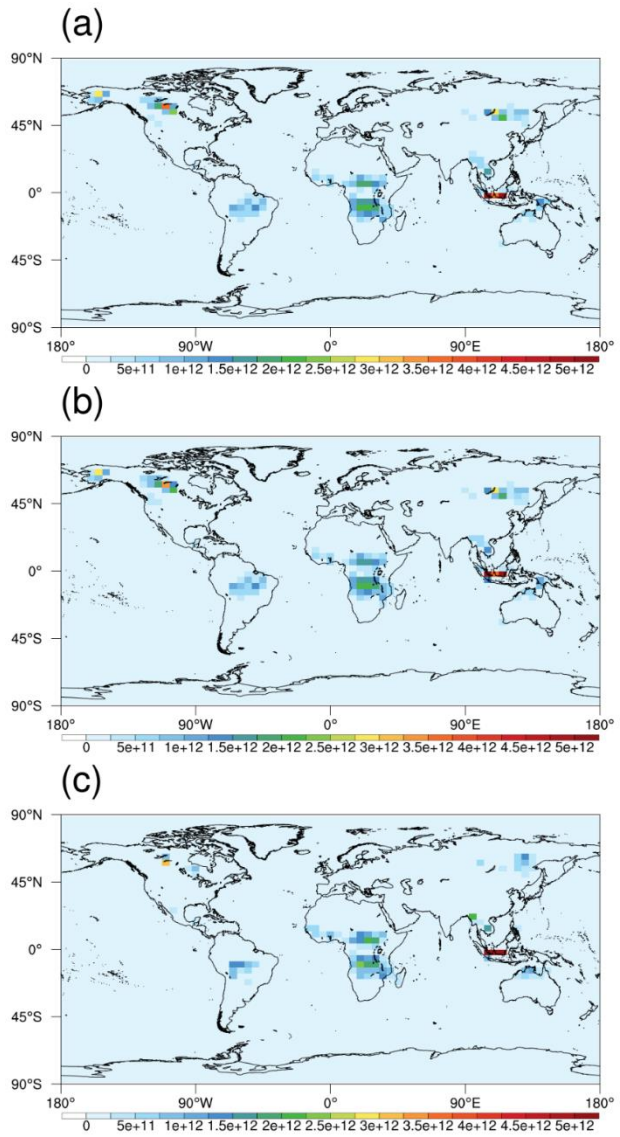

Fig. S6. GFED4 CO emissions in 2015 from (a) GC-v12; (b) GC-Adjoint-HEMCO; and GFED3 CO emissions in (c) GC-Adjoint-STD. The unit is molec/cm2/s.

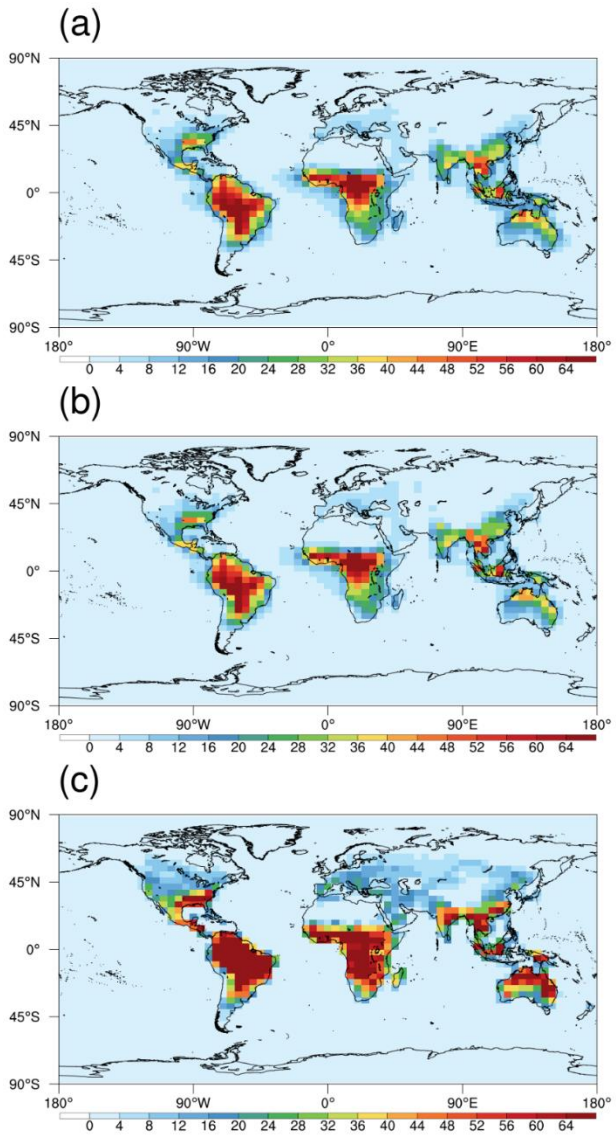

Fig. S7. PCO_NMVOC columns from (a) GC-v12; (b) GC-Adjoint-HEMCO; (c) GC-Adjoint-STD in 2015. The unit is kg/s.

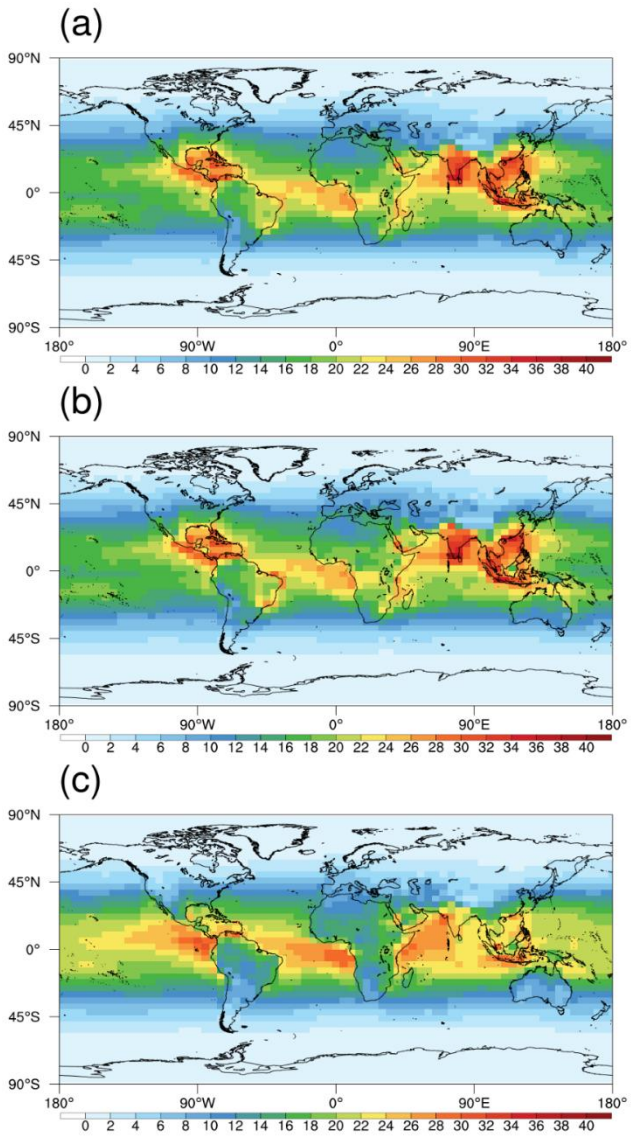

Fig. S8. PCO_CH4 columns from (a) GC-v12; (b) GC-Adjoint-HEMCO; (c) GC-Adjoint-STD in 2015. The unit is kg/s.

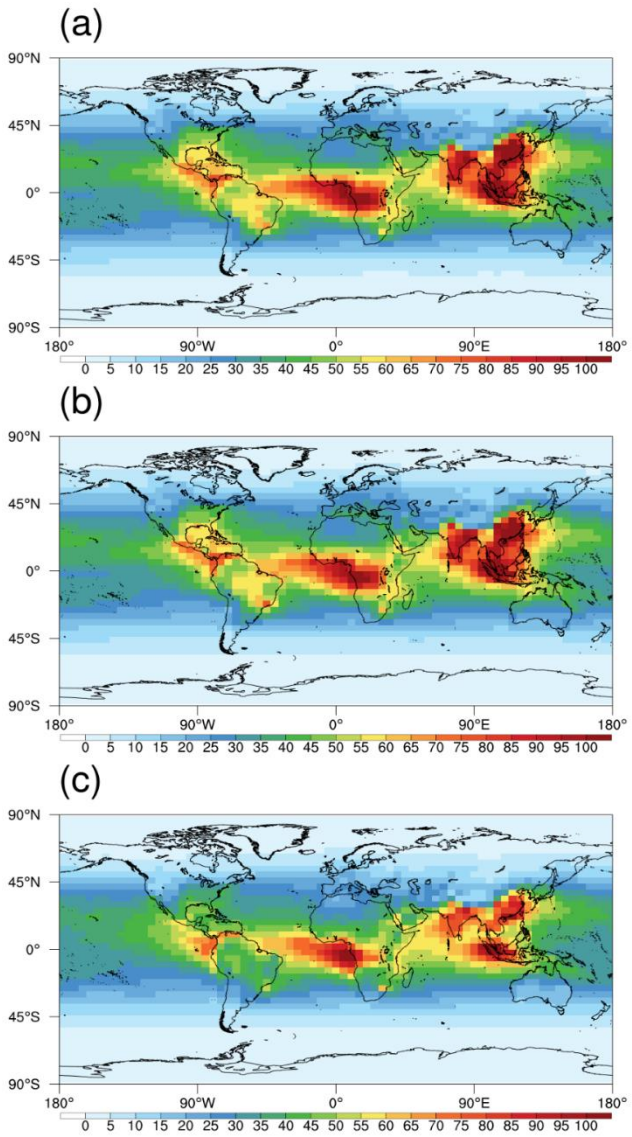

Fig. S9. CO_OH columns from (a) GC-v12; (b) GC-Adjoint-HEMCO; (c) GC-Adjoint-STD in 2015. The unit is kg/s.

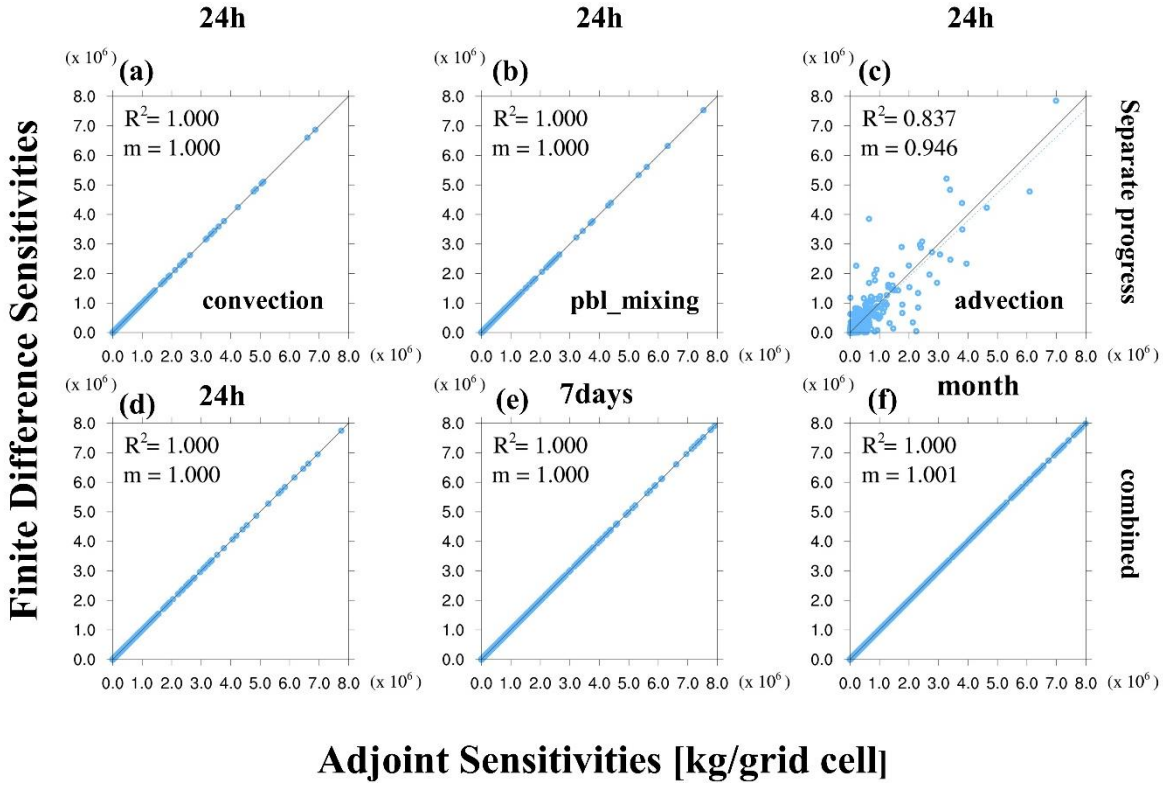

Fig. S10. Comparison of sensitivities of global CO concentrations (LFD_GLOB and model level 5) to CO emission scaling factors calculated using the adjoint method vs. the finite difference method. (a-c) the effects of convection, PBL mixing and advection with 24-hour assimilation window; (d-f) the combined effects (the advection process is turned off) with increased assimilation windows.

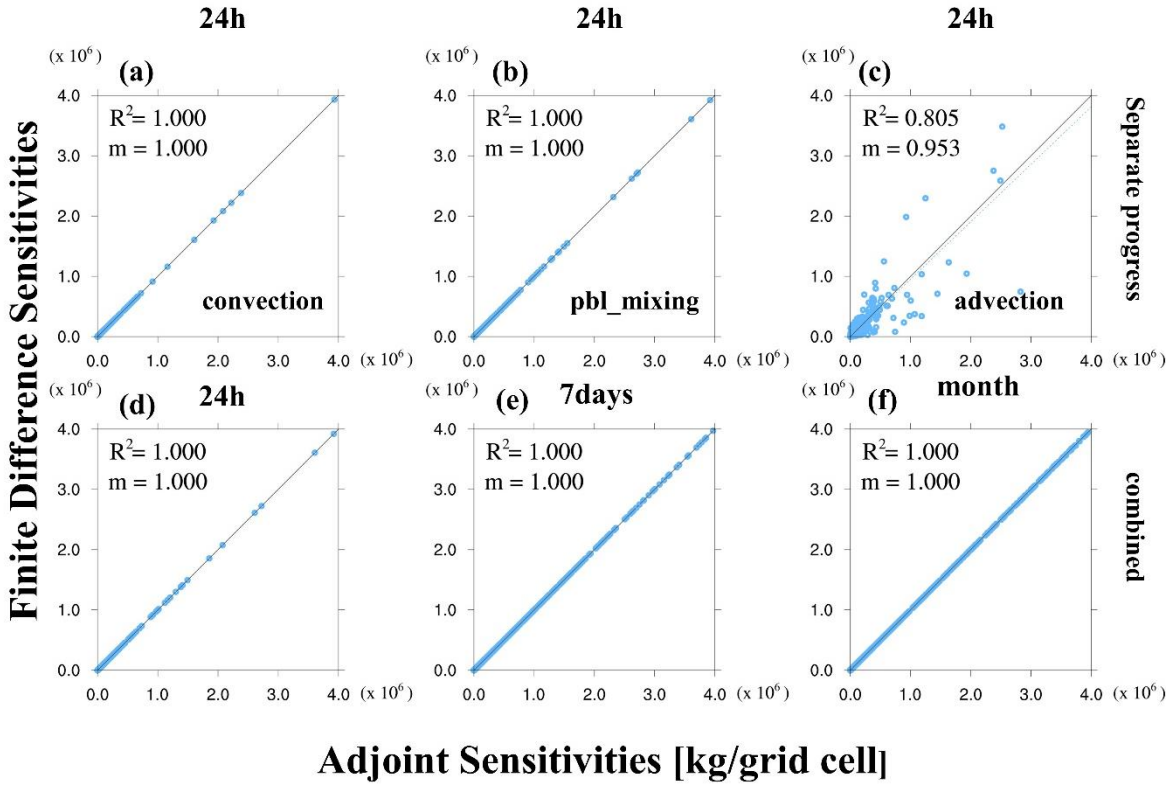

Fig. S11. Comparison of sensitivities of global CO concentrations (LFD_GLOB and model level 15) to CO emission scaling factors calculated using the adjoint method vs. the finite difference method. (a-c) the effects of convection, PBL mixing and advection with 24-hour assimilation window; (d-f) the combined effects (the advection process is turned off) with increased assimilation windows.