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Extreme weather exacerbates ozone pollution in the Pearl River Delta, China: role of natural processes

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Supporting Information

Supporting Information includes 14 pages, 11 figures and 4 tables

SI Figures S1-S11

SI Tables S1-S4

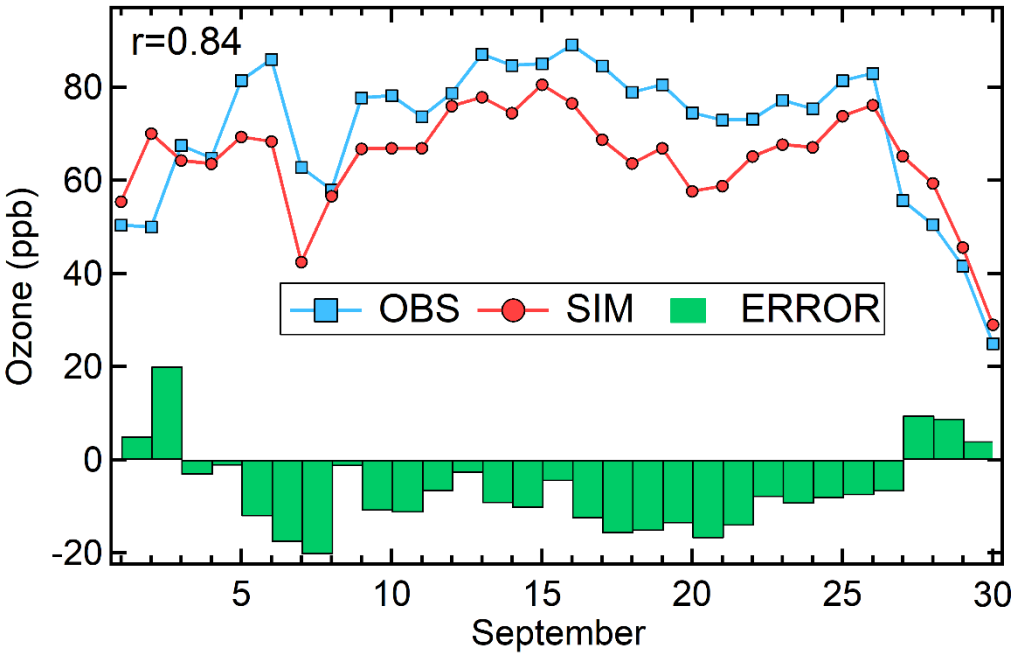

Figure S1 Validation of the stepwise regression model

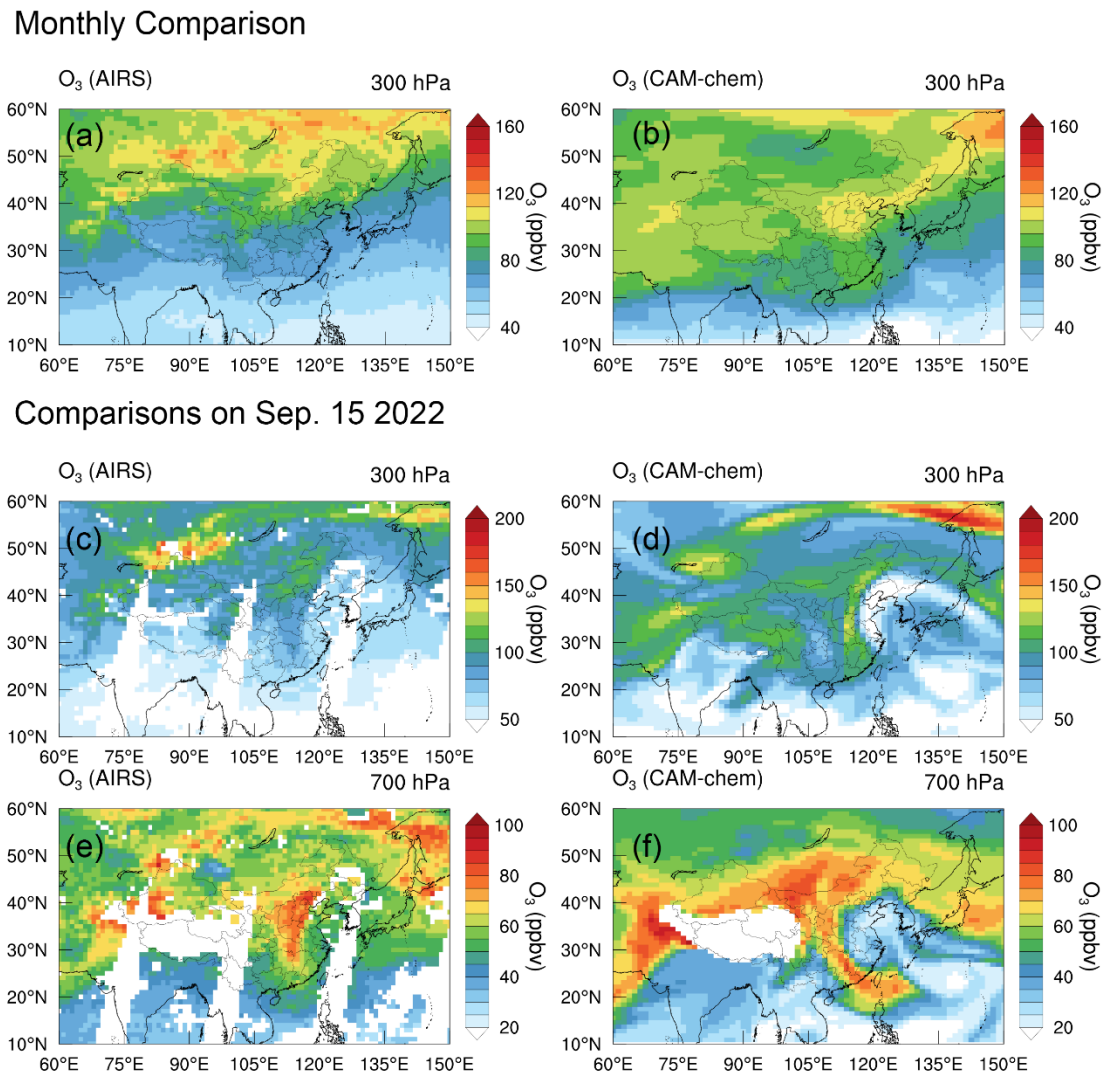

Figure S2 Comparisons of CAM-Chem simulated O3 and satellite retrieved O3 from AIRS. (a) and (b) distribution of monthly averaged O3 levels at 300hpa; (c) and (d) distribution of 300 hpa O3 levels on Sep. 15 2022 (illustrating the STE event); (e) and (f) same as (c) and (d) but at 700 hpa.

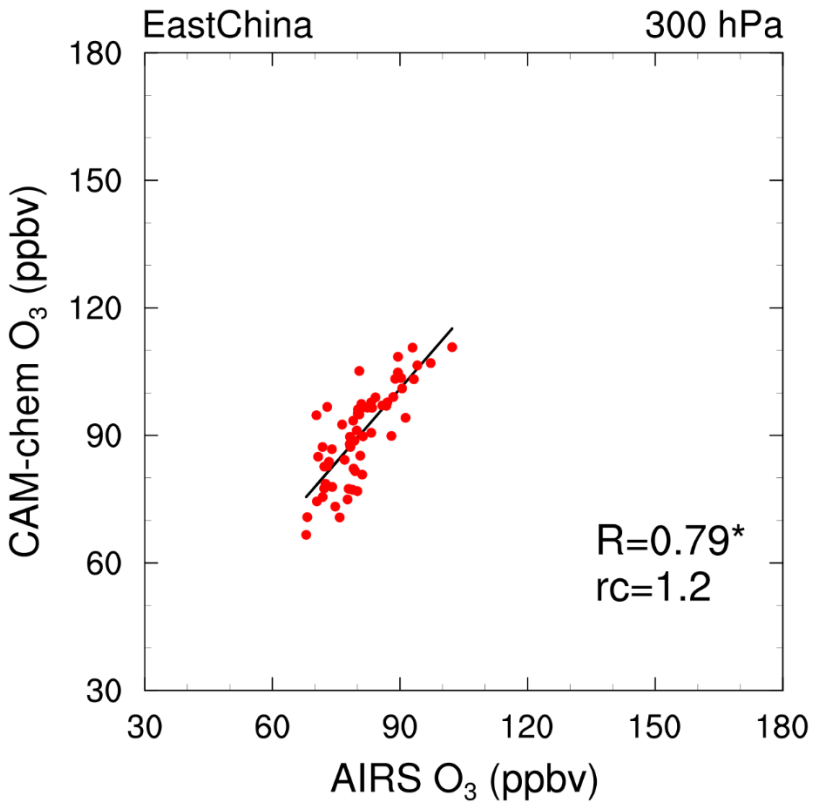

Figure. S3 Validation of AIRS O_3 and CAM-Chem simulated O_3 at 300hPa in Eastern China (R indicates correlation coefficient; rc indicates regression coefficient)

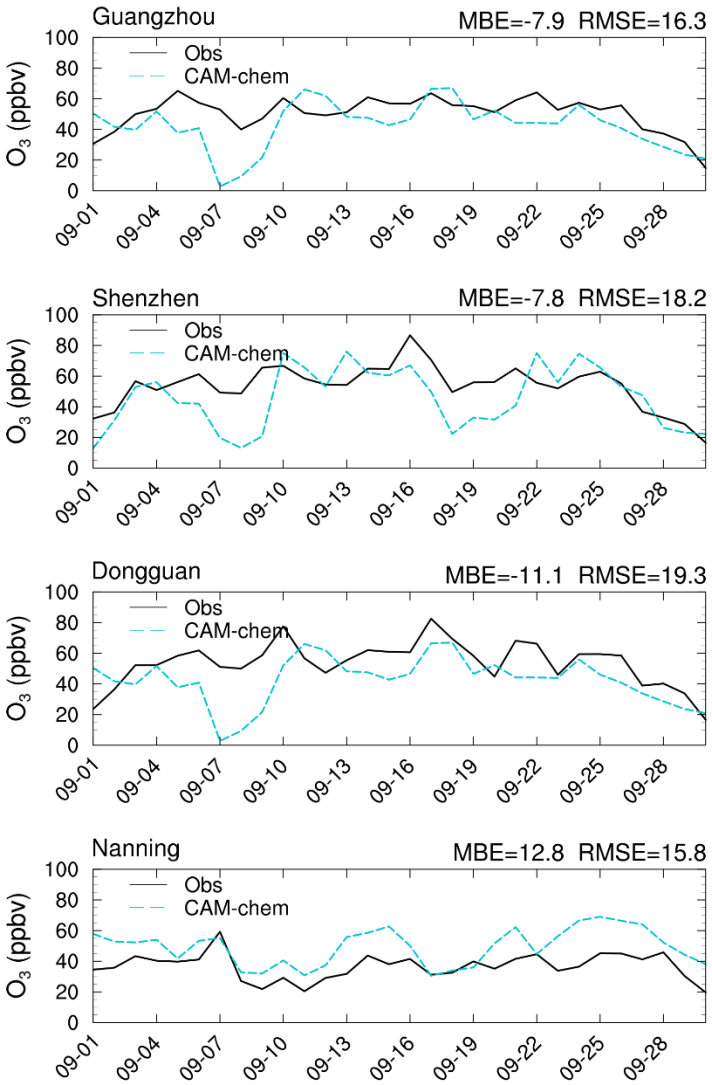

Figure S4 Comparisons of the CAM-Chem performance with surface monitrong O3 concentrations (MBE stands for mean bias error and RMSE stands for root mean square error. Obs refers to data from observations and CAM-Chem refers to the model simulated result.)

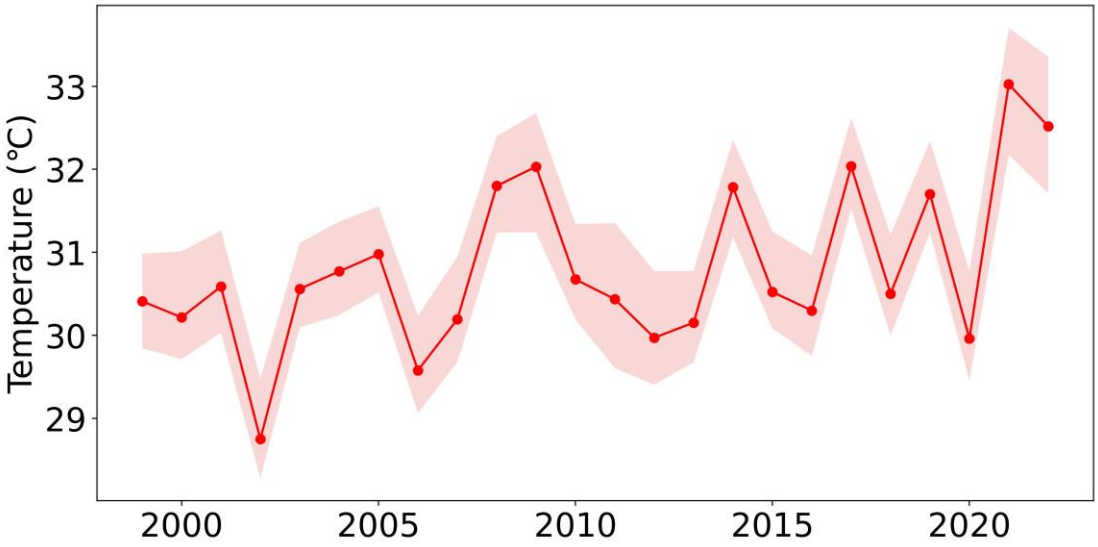

Figure S5 Historical variation of monthly average daily-maximum temperature in PRD in September from 1999 to 2022

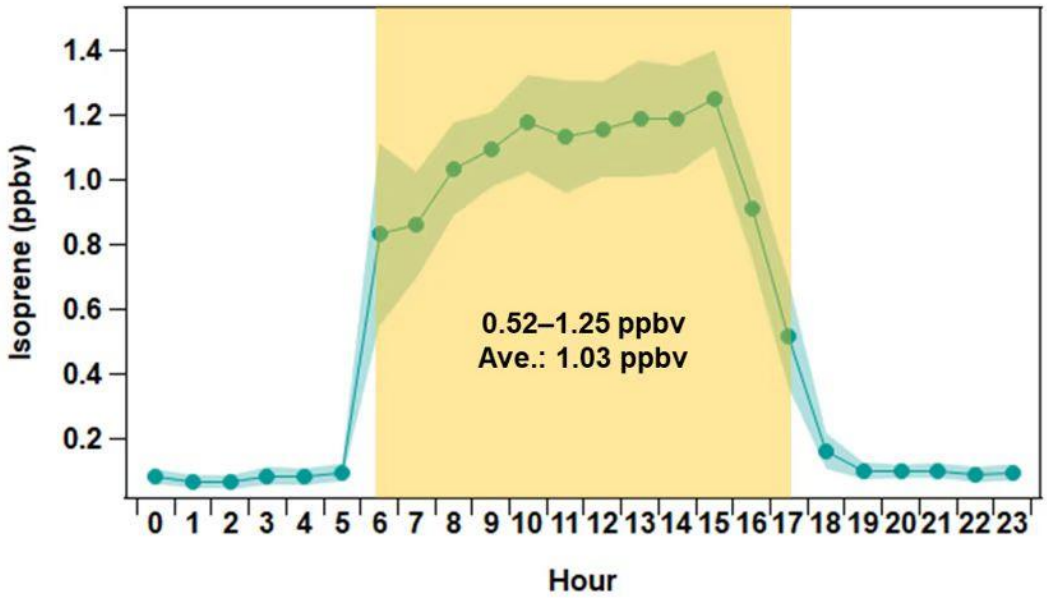

Figure S6 Diurnal variation of isoprene concentrations at HZ Base. (The yellow shaded highlights the daytime averaged concentrations, 0.51-1.25 ppbv. The daily averaged concentration was 1.03 ppbv.)

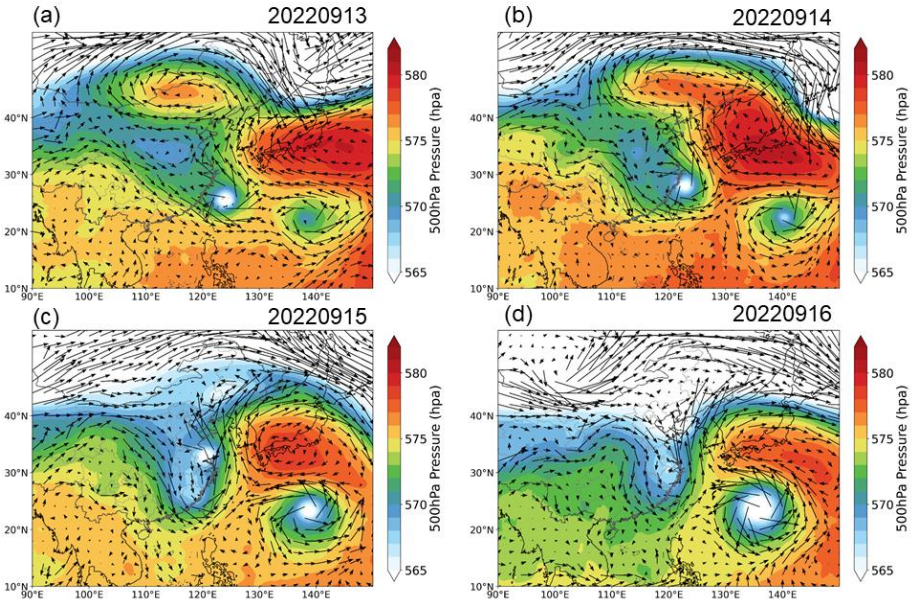

Figure S7 Synoptic weather from September 13 to September 16 2022

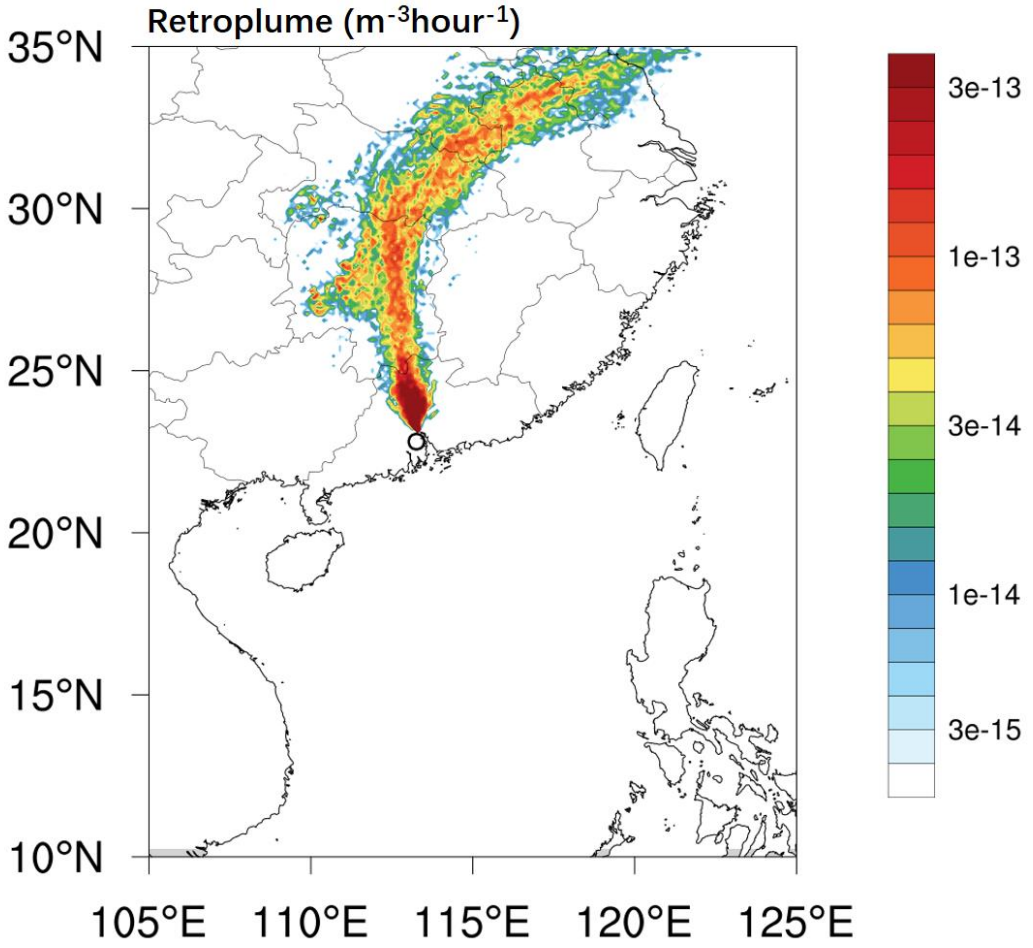

Figure S8 LPDM simulated 48h retroplume (footprint residence time) showing transport pathways of air masses impacting PRD

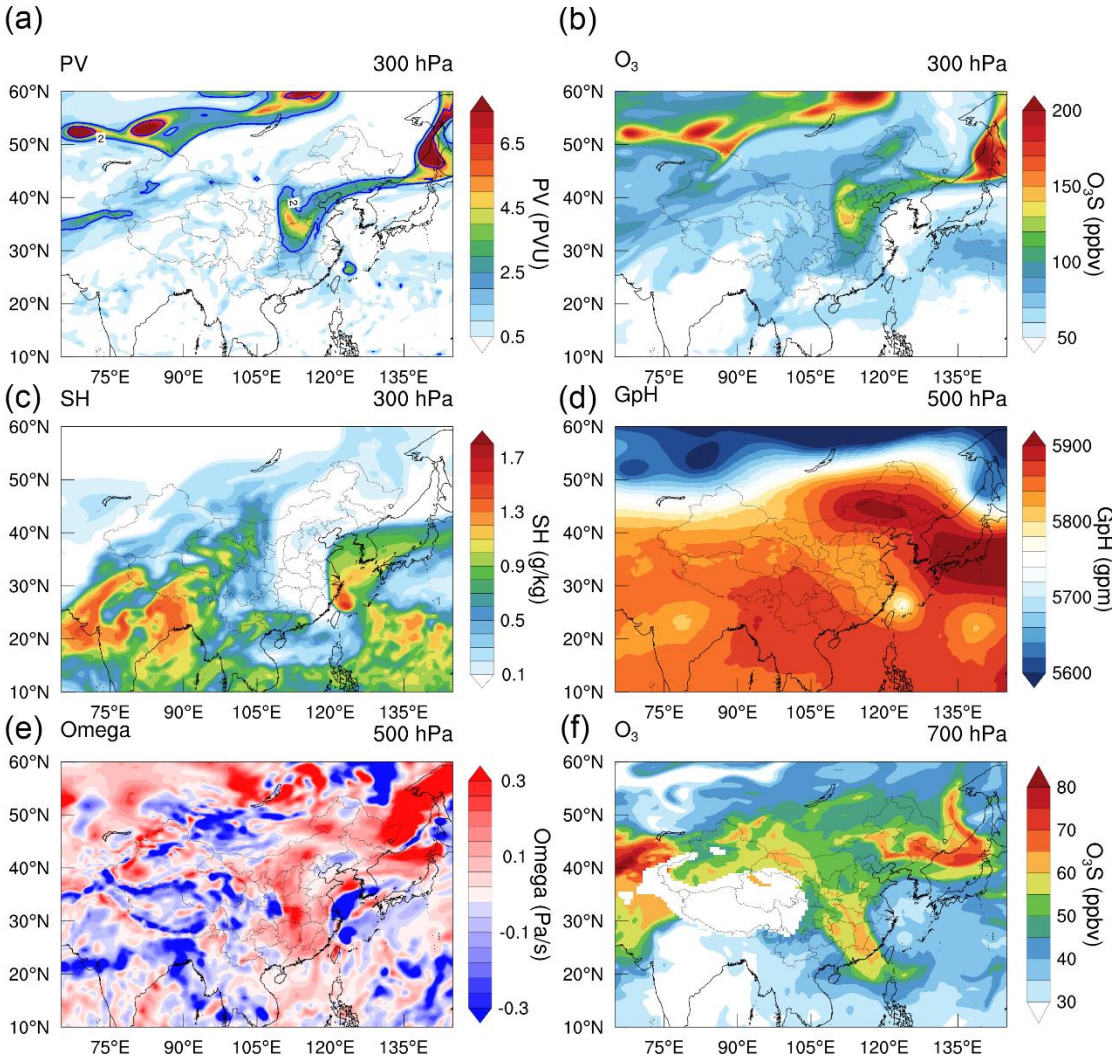

Figure S9 Evidence illustrating STE O_3 intrusion on September 13, 2022. (a) Spatial distribution of potential vorticity (PV) at 300hPa over China (The blue solid line indicates the dynamical tropopause of 2PVU, 1 PVU=10^{-6} m^2 s^{-1} K kg^{-1}); (b-e) The distribution of O_3 concentration (at 300 hPa), specific humidity (at 300 hPa, SH), geopotential height (at 500 hPa, Gph), vertical velocity (at 500 hPa, Omega), and O_3 concentration (at 700 hPa), respectively. All the data were identified based on ERA5 database.

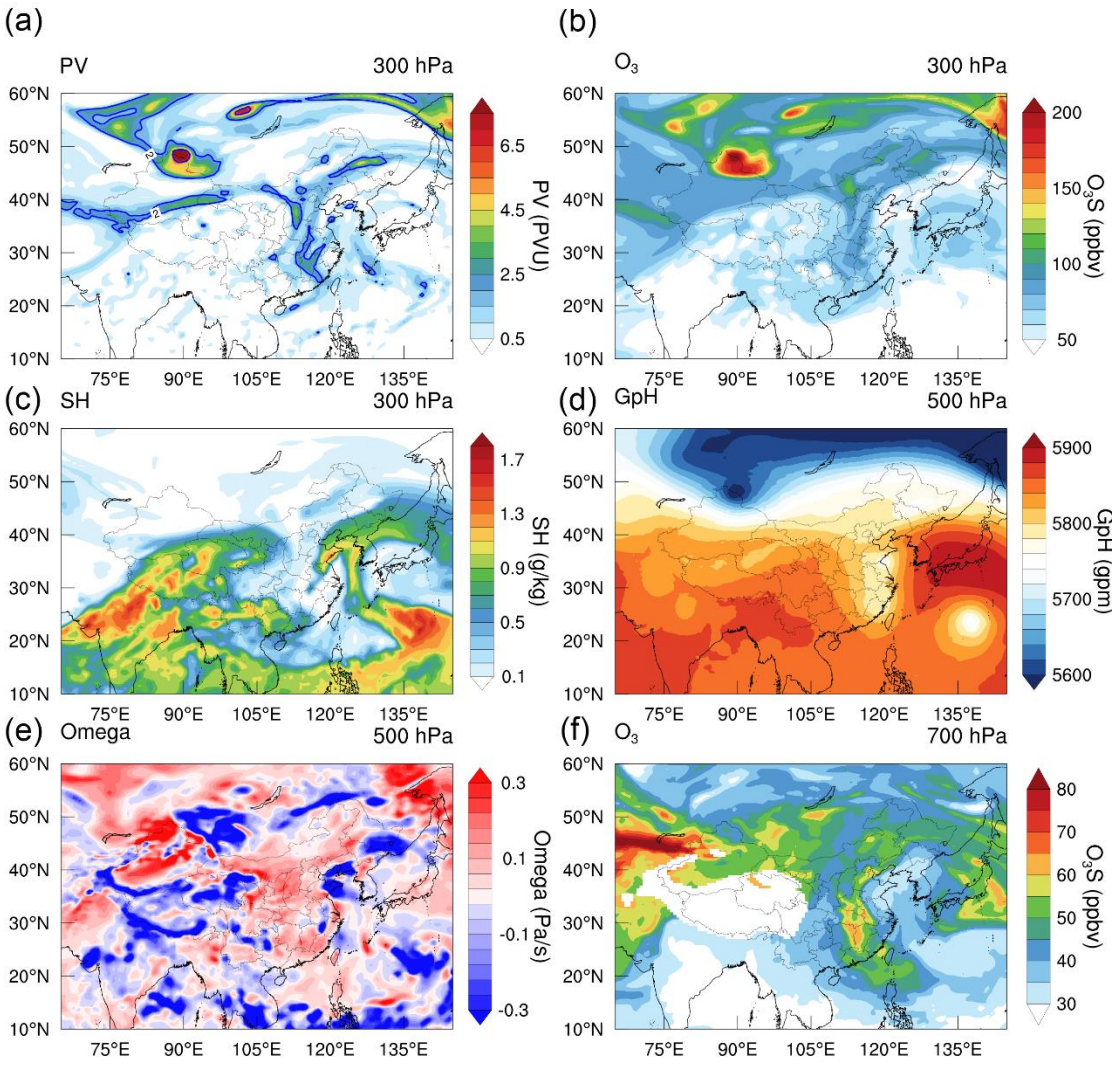

Figure S10 Same as Fig S9 but on September 15

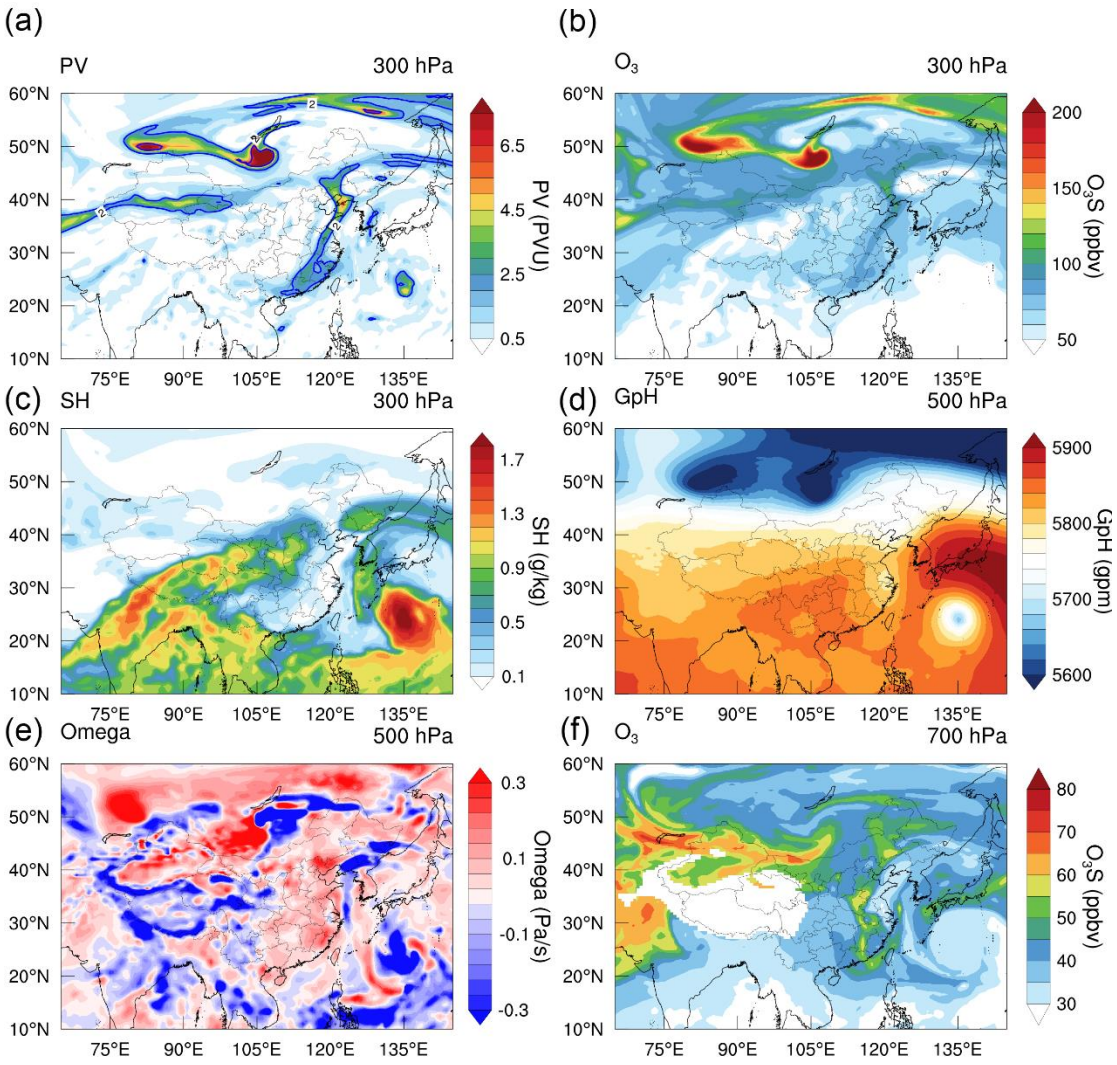

Figure S11 Same as Fig S9 but on September 16

Table S1 Introduction of monitoring instruments used in this work

Parameter	Manufacture	Model	Resolution
O_3	Thermo Scientific	49i-D1NAA	5min
NOx	Thermo Scientific	42i-DNMSDAA	5min
CO	Thermo Scientific	48i-DNSAA	5min
SO_2	Thermo Scientific	43i-DNSAA	5min
VOC	AMA, Germany	GC5000-FID	1h

Table S2 Configuration and settings of WRF-CMAQ modeling system

Item	Scheme
Grid resolution	12×12 km
Initial/boundary conditions	WRF: NCEP FNL reanalysis data CMAQ: Mother domain (36k×36km grid resolution)
Microphysics	WRF single-moment 5-class microphysics
Short-wave radiation	Goddard
Long-Wave radiation	RRTM
WRF nudging	Yes
Boundary Layer	ACM2
Gas-phase Chemistry	CB05
Aerosol option	AERO5
Dry deposition	M3DRY
Anthropogenic emissions	MEIC
Natural emissions	MEGAN

Table S3 WRF-CMAQ Model performance of O_3, and NO_2 in Guangzhou

Variables	O_3 (ppb)*	NO_2 (ppb)*
MB	-8.08	1.76
NME	-0.28	0.11
RMSE	27.74	9.42
IOA	0.74	0.72

*The WRF-CMAQ simulated O_3 and NO_2 were validated with observed O_3 and NO_2 in Guangzhou using statistical metrics (MB stands for mean bias, NME stands for normalized mean bias, RMSE stands for root mean square error and IOA stands for index of agreement)

Table S4 The recorded tropical cyclones influencing PRD in September 2022

Name	Start time	End time	Max intensity
Hinnamnor	Aug 27	Sept 8	SuperTY*
Muifa	Sept 6	Sept 16	STY**
Nanmadol	Sept 12	Sept 20	SuperTY
Noru	Sept 21	Sept 29	SuperTY

*SuperTY refers to super typhoon

**STY refers to severe typhoon. The classification was based on China Grade of tropical cyclones (GB/T 19201-2006)