

Evaluations of Hourly PM Mass and Species Simulations by Models-3/CMAQ

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Introduction

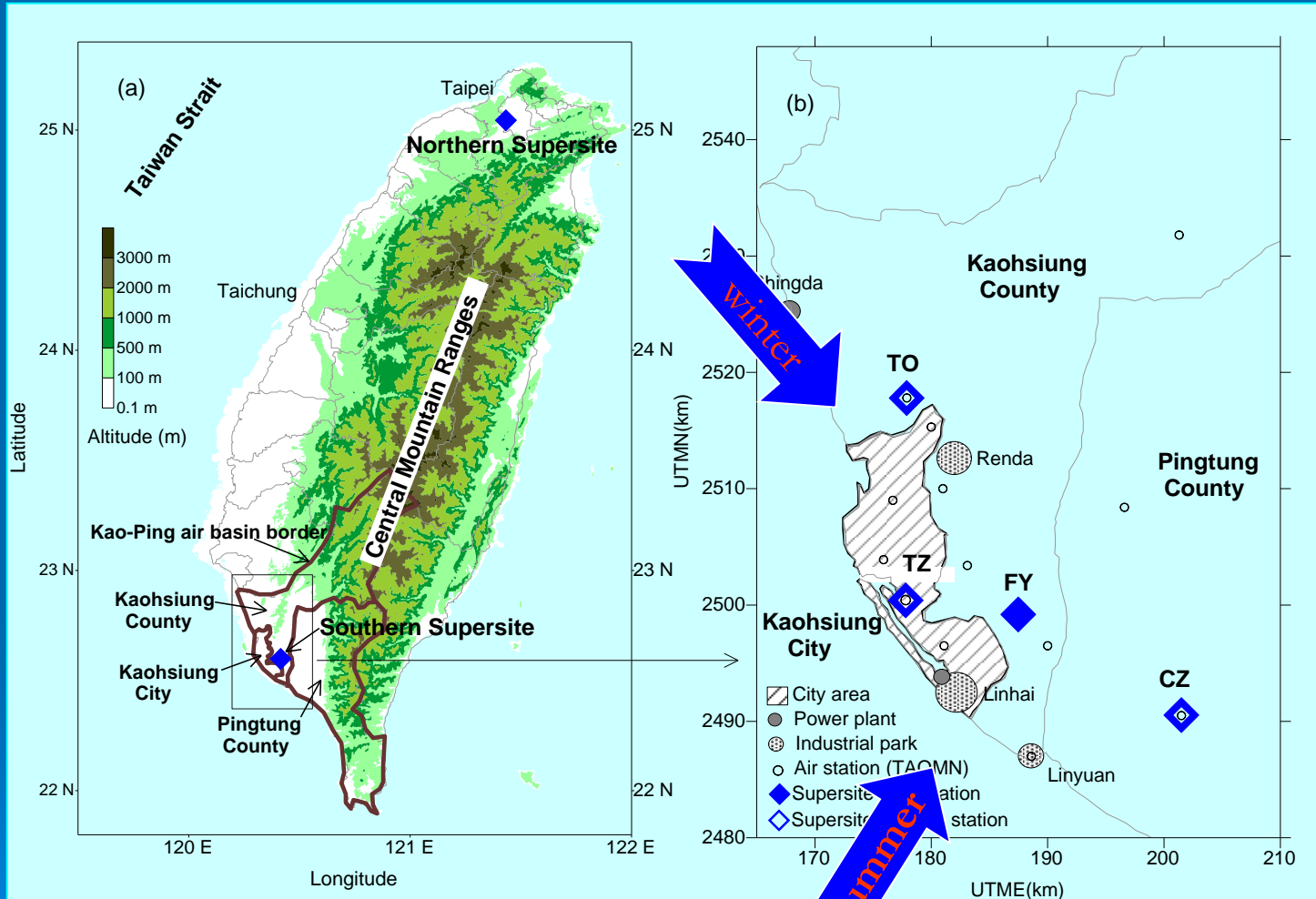
Model evaluation for PM simulation is based on 24-hour average concentrations for PM mass and species concentrations;

Model outputs and measurements are generally hourly concentrations.


	配對值絕對偏差	配對值常化偏差
PM ₁₀	< 150%	-50% ~ 80%
NO _x	< 80%	-40% ~ 50%
SO ₂	< 80%	-40% ~ 50%

Model evaluations based on hourly data are more scientifically correct.

Locations of Southern Taiwan Supersites



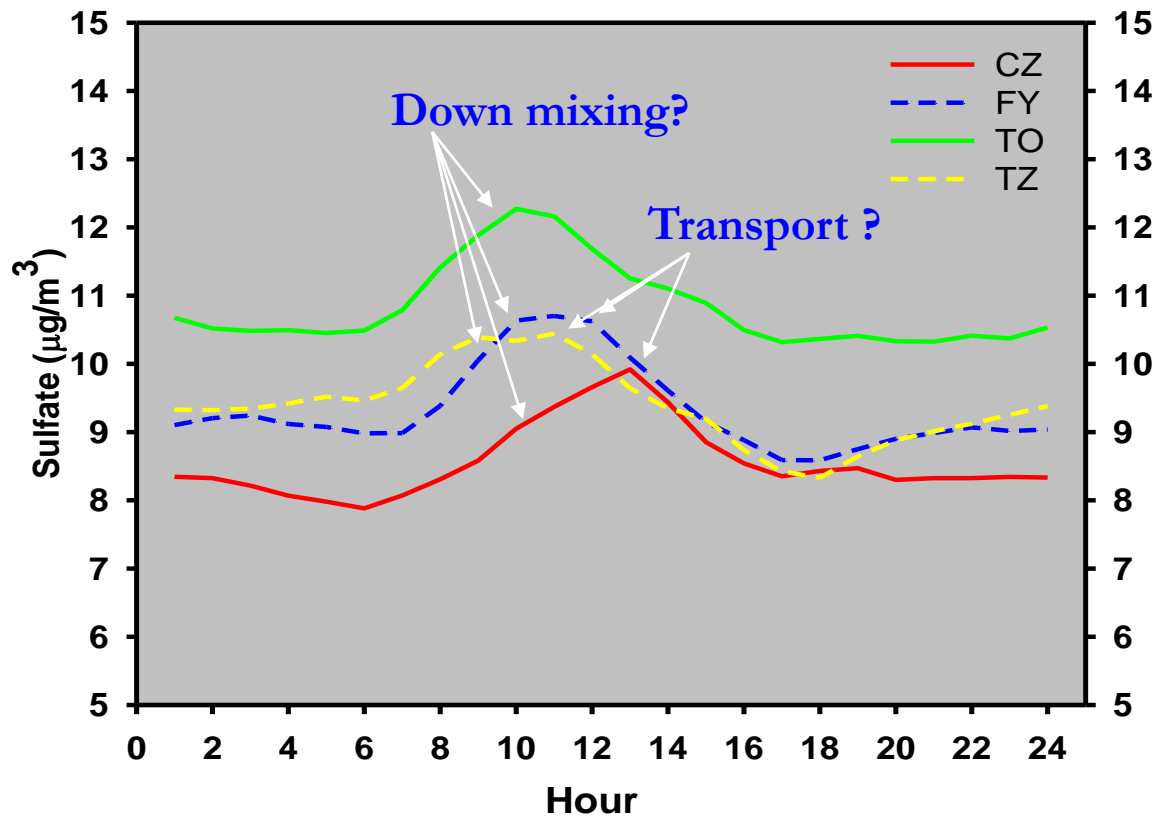
Purposes of Southern Taiwan PM Supersites Study

- To characterize the ambient PM concentrations, size distributions, and chemical compositions;
 - To study the formation pathways of PM;
 - To formulate control strategies/measures.
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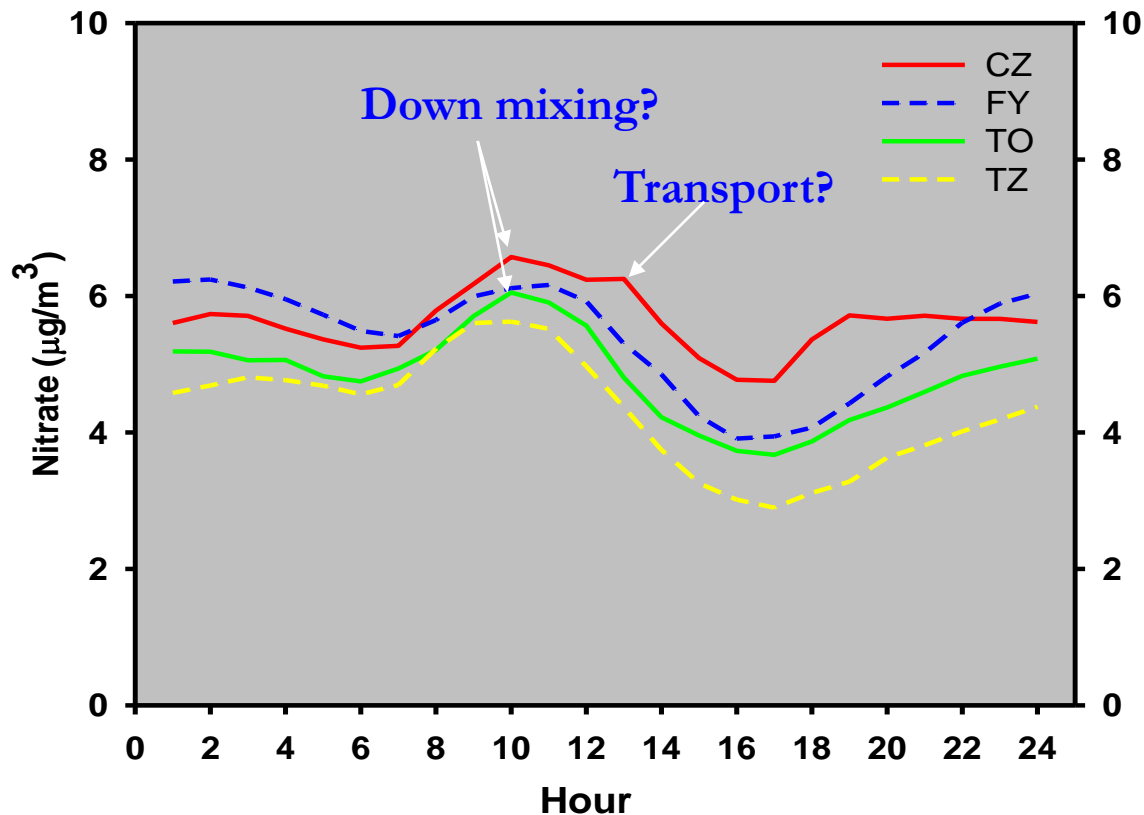
Measurement Methods

Species	Measurement Method
SO ₂	UV fluorescence
NO _x	Chemiluminescence
O ₃	UV absorption
PM	RP1400
Nitrate	RP8400N
Sulfate	RP8400S
OC/EC	Sunset 5040
H ₂ O ₂	AL-2021
HNO ₃	RP3500 (Denuder)

Comparison of diurnal variations at different sites (Sulfate)

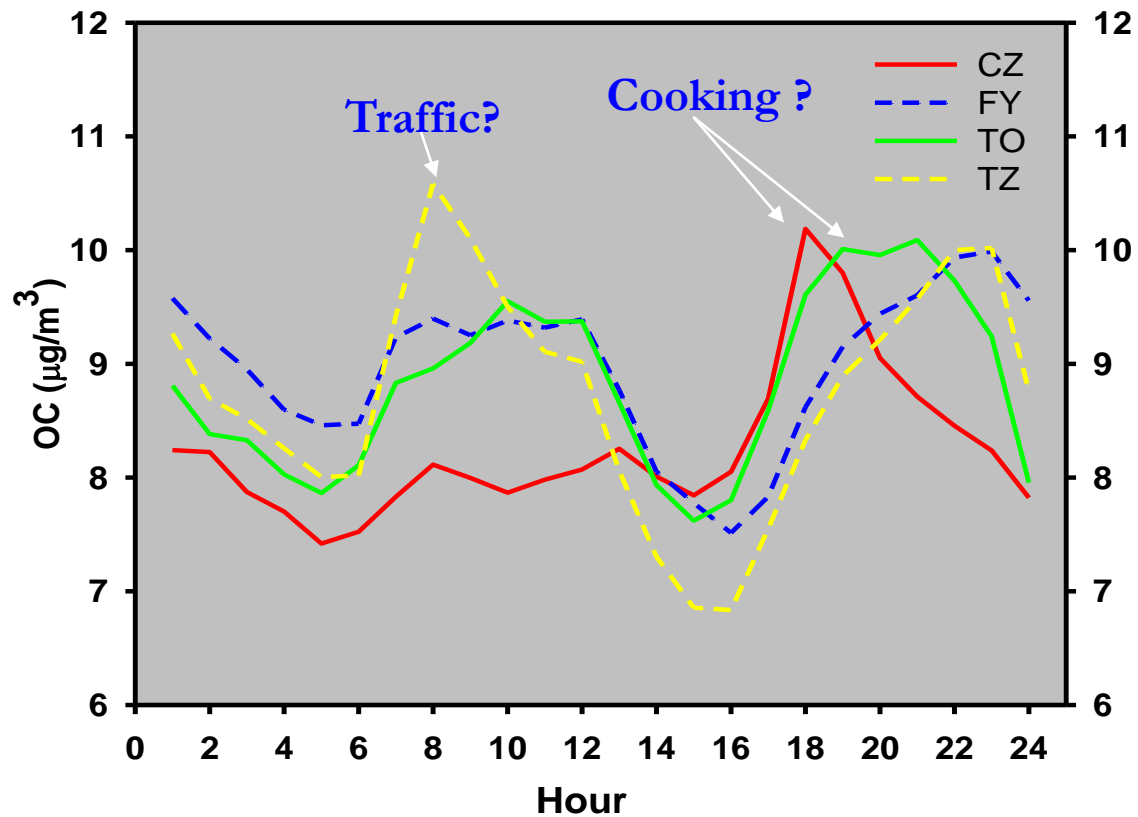


Comparison of diurnal variations at different sites (Nitrate)

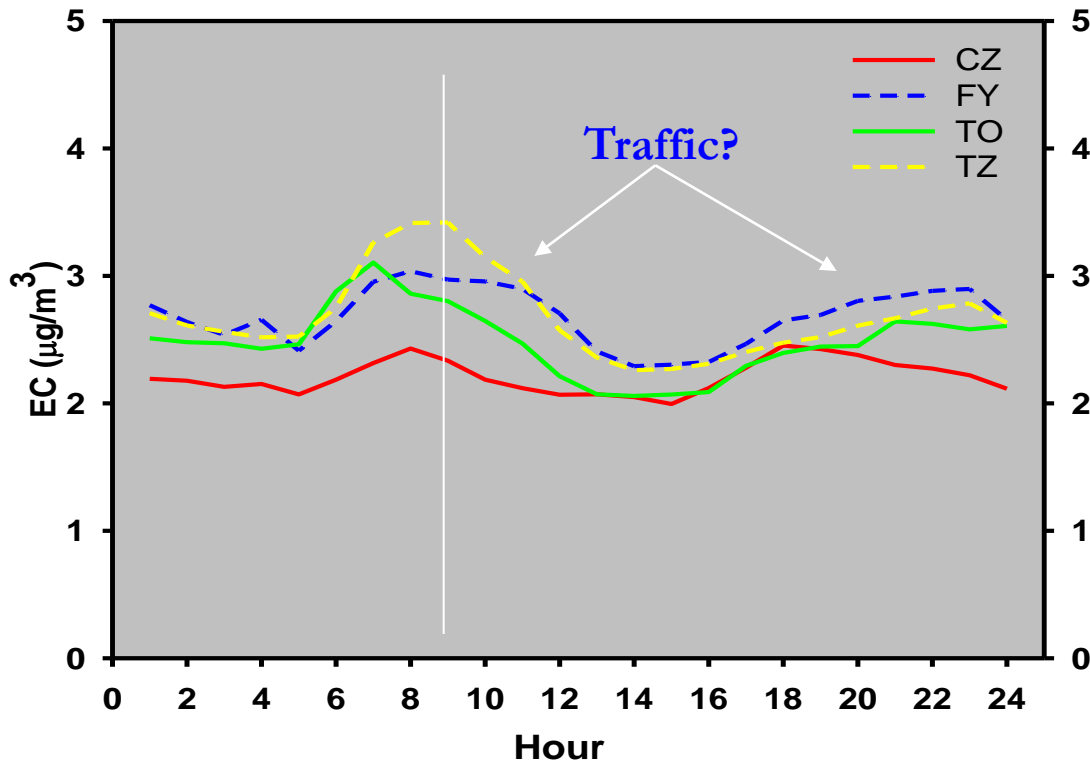


Bottom line: (1) CZ peak different from other stations could be resulted from transport

Comparison of diurnal variations at different sites (OC)



Comparison of diurnal variations at different sites (EC)



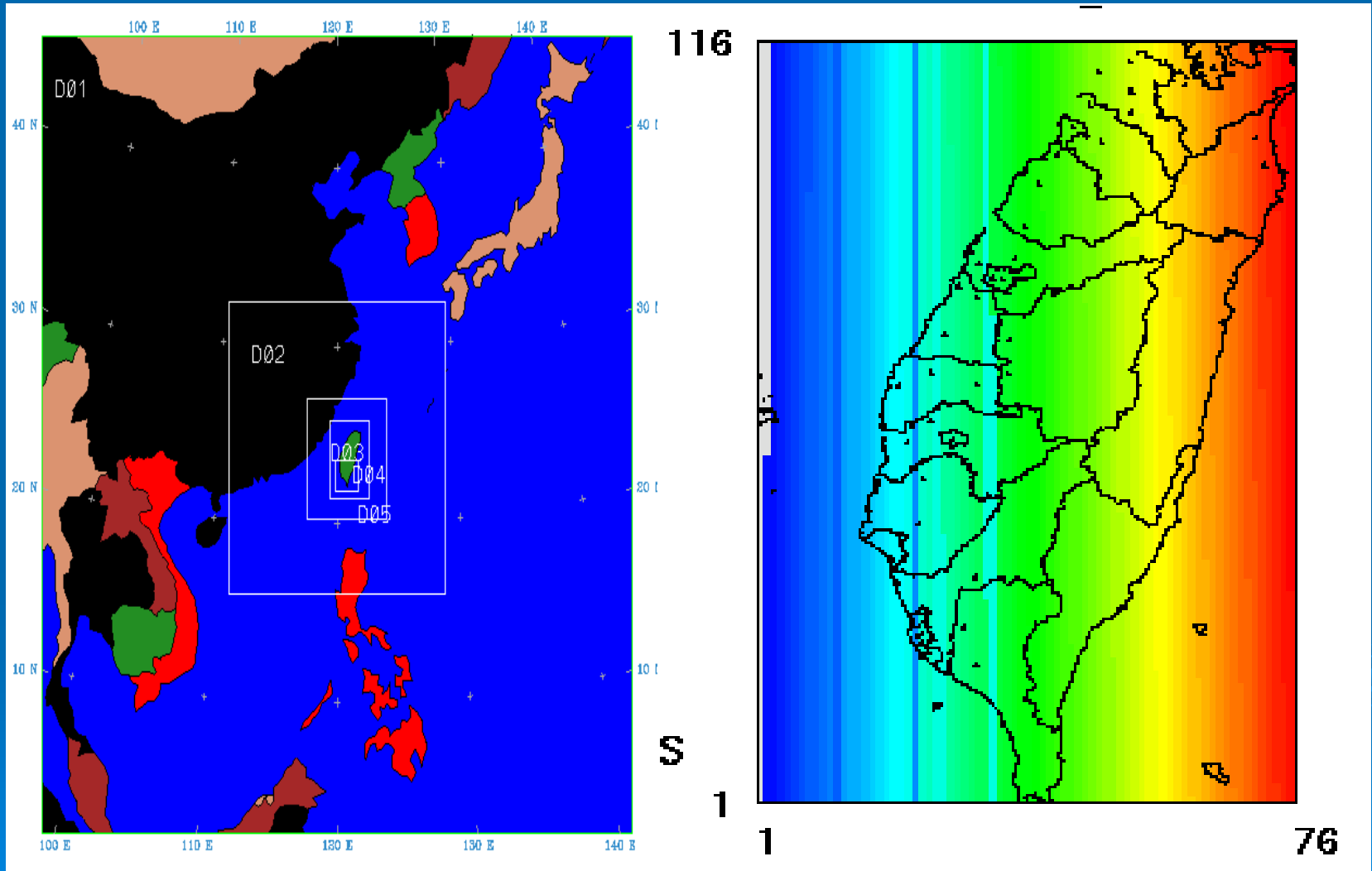
Bottom line: (1) All sites peak at 7-9 h in the morning indicating traffic related.

CMAQ Modules

- **Meteorology : MM5 with MCIP**
- **Vertical layers: 24 in MM5 and 15 in CCTM**
- **Chemistry : CB-IV**
- **Aerosol : Aerosol module version 3**
- **Simulation periods: 2005/11/01-05**

Heterogeneous HONO formation mechanism added

Simulation Domains



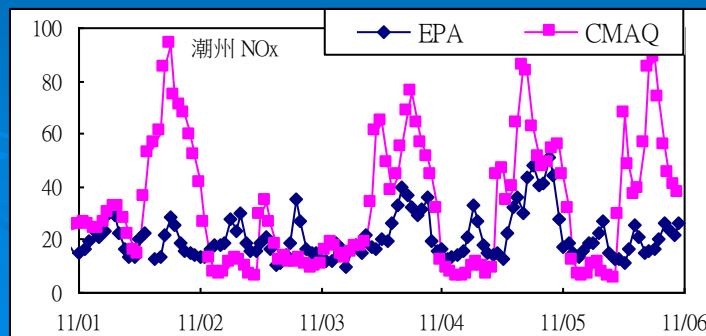
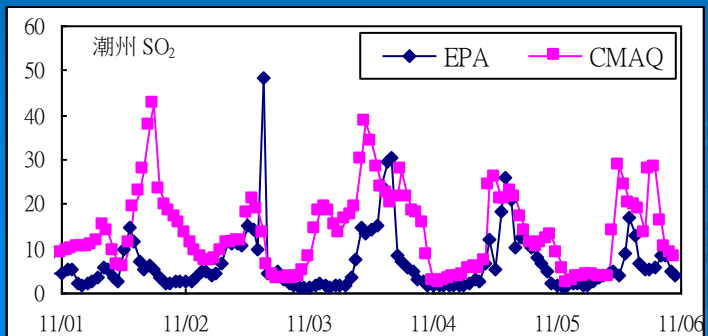
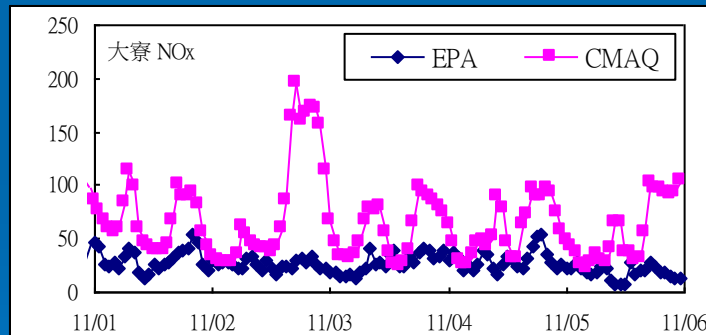
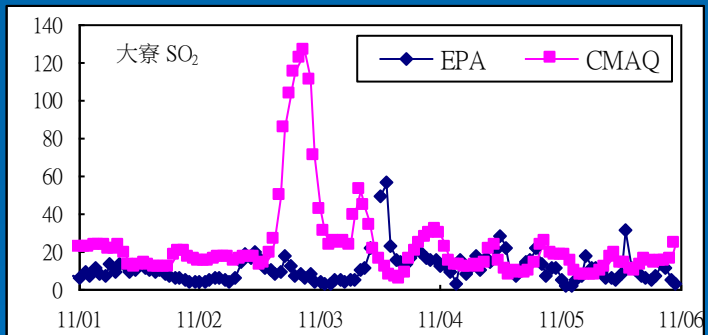
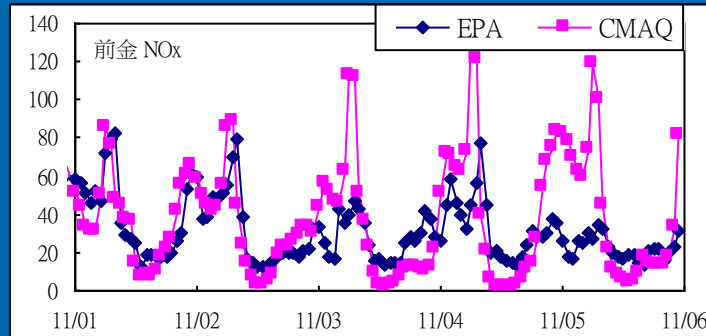
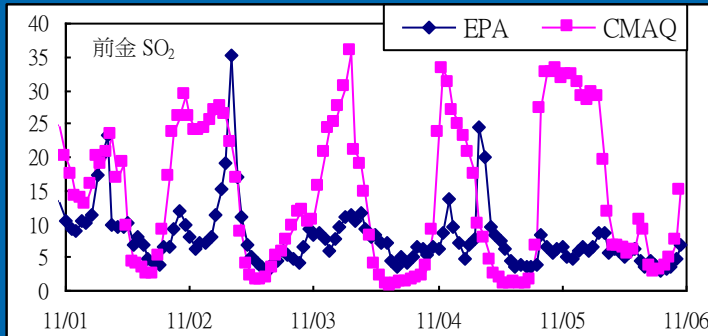
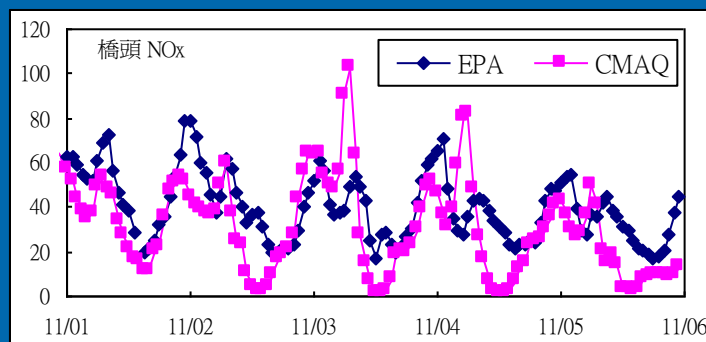
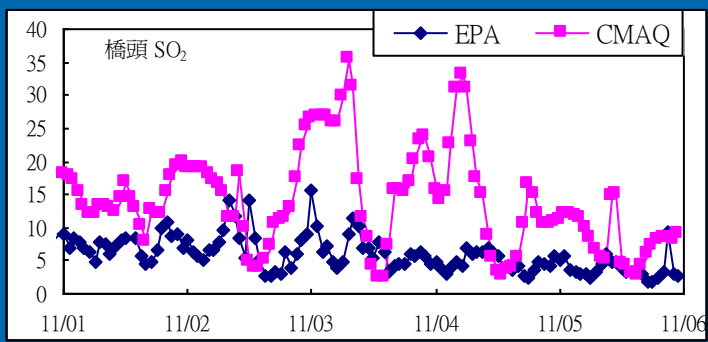
4 layers nesting to 3 km by 3 km

Sigma-layer

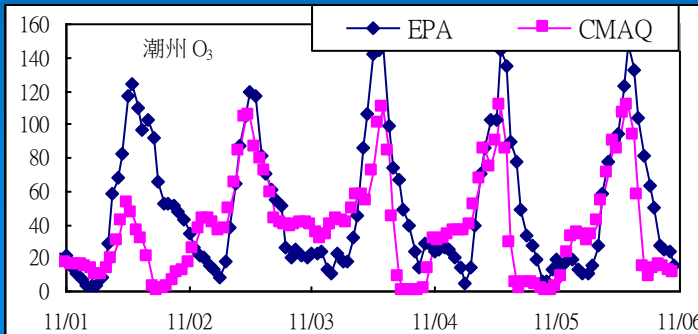
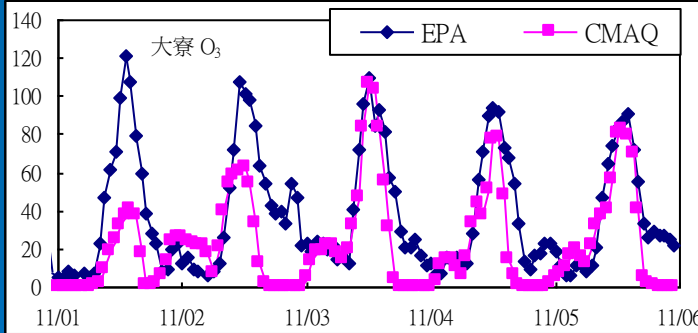
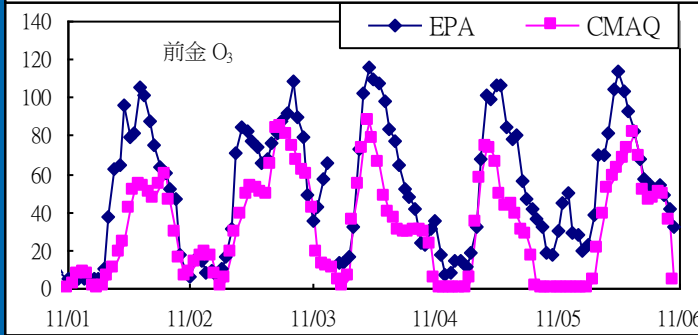
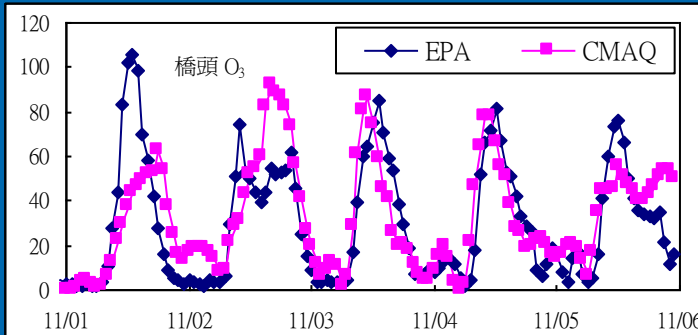
Layer	Sigma	Pressure (Pa)	Height (m)	Half Range (m)
15	0.000	10000	21146	17223
14	0.150	23500	13300	10688
13	0.350	41500	8077	6784
12	0.500	55000	5490	4794
11	0.600	64000	4099	3494
10	0.700	73000	2890	2616
9	0.750	77500	2341	2082
8	0.800	82000	1823	1577
7	0.850	86500	1332	1145
6	0.890	90100	957	777
5	0.930	93700	598	467
4	0.960	96400	337	252
3	0.980	98200	167	125
2	0.990	99100	83	62
1	0.995	99550	41	21
0	1.000	100000	0	

SO₂

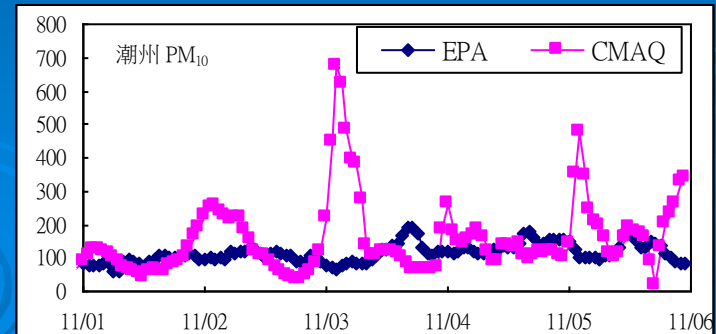
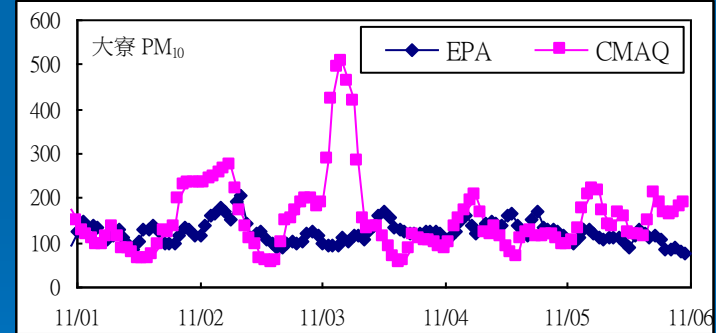
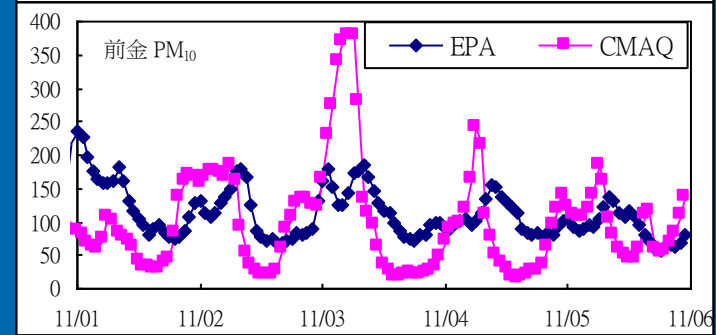
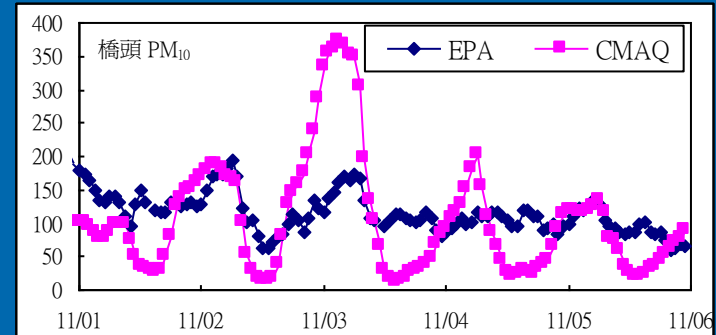
NO_x



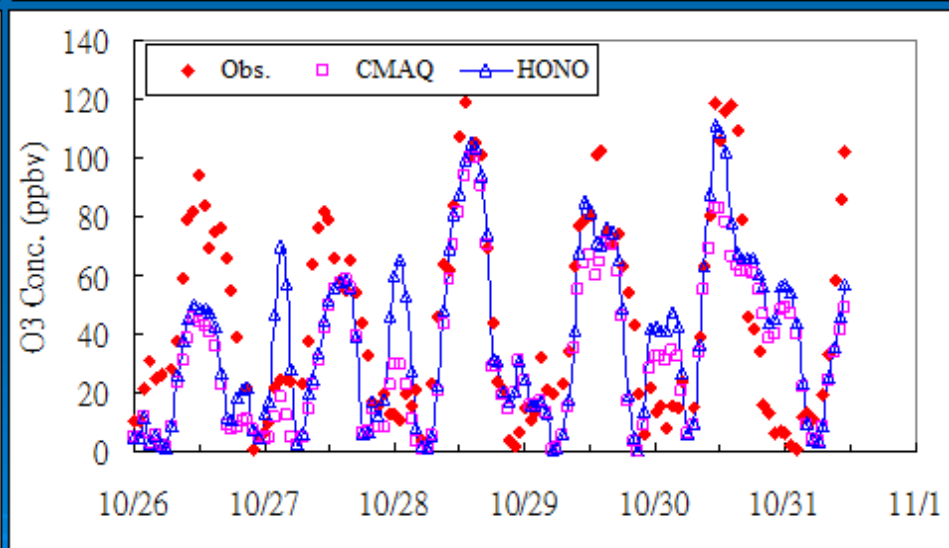
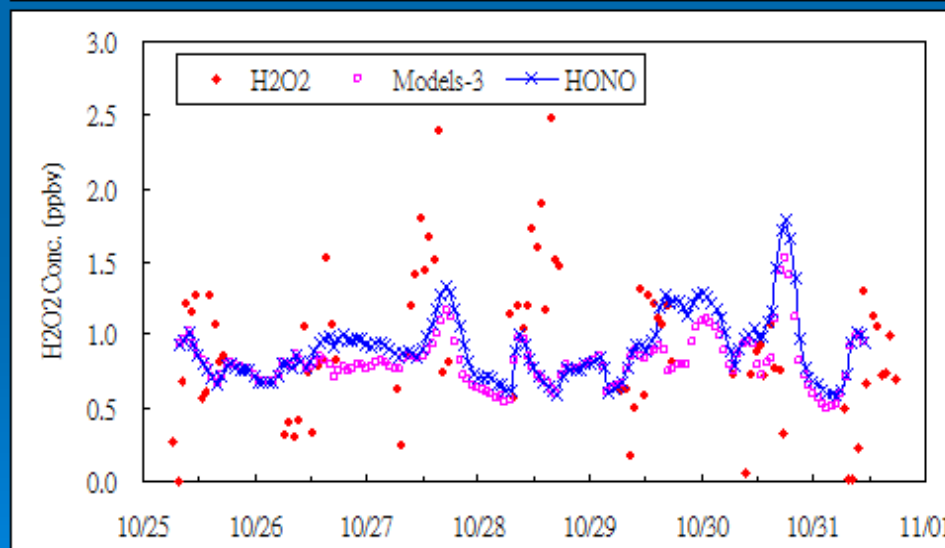
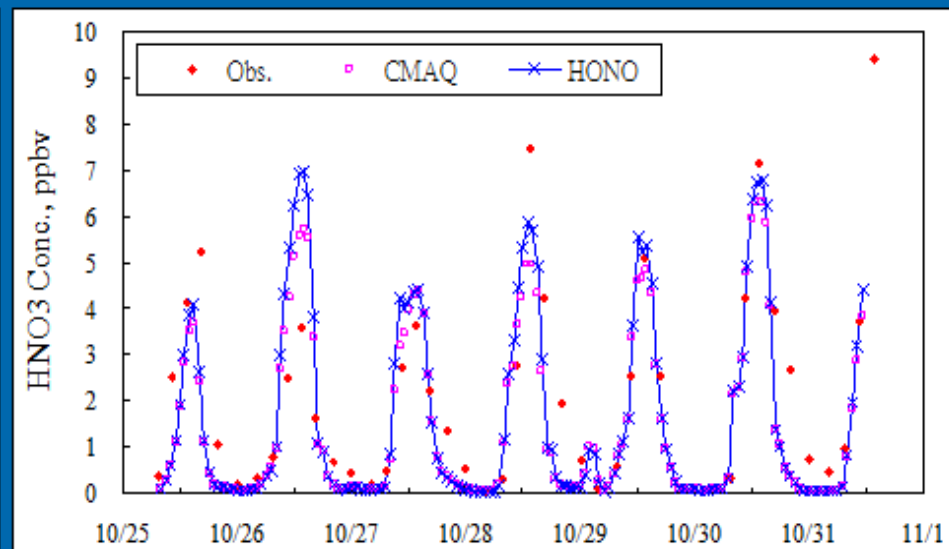
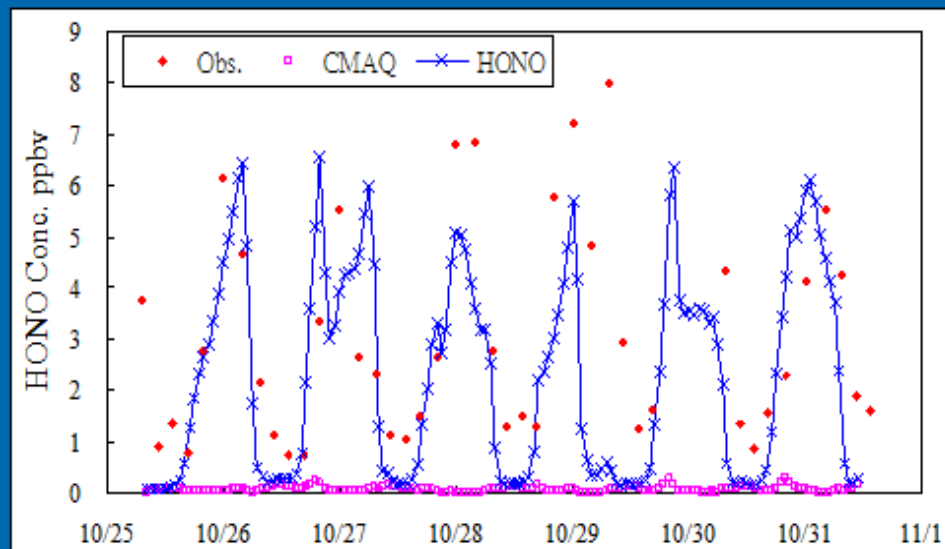
O₃



PM

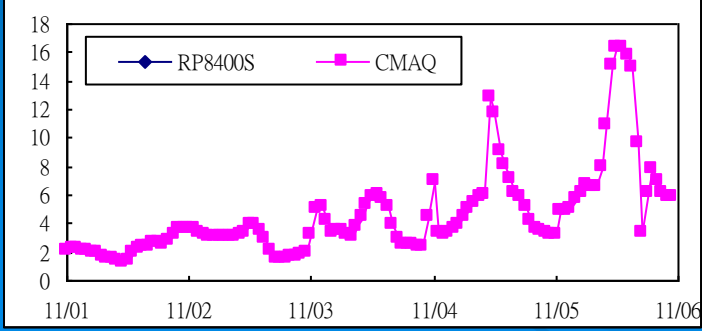
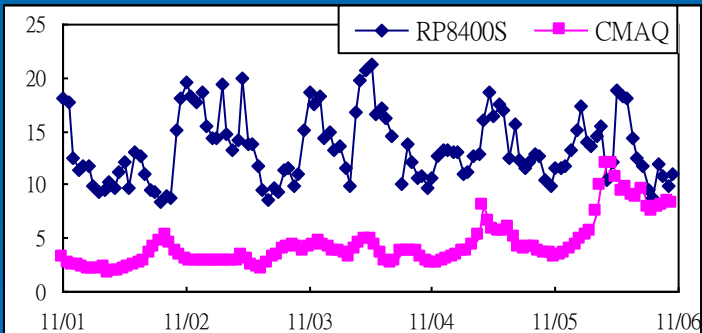
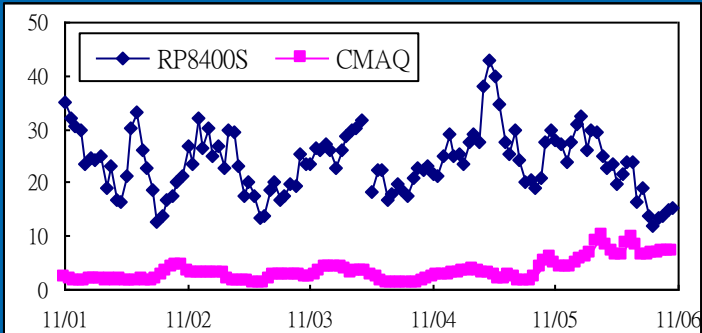
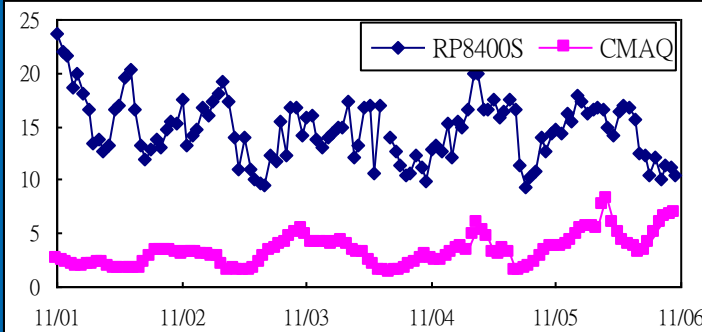


Modifications of HONO Formation

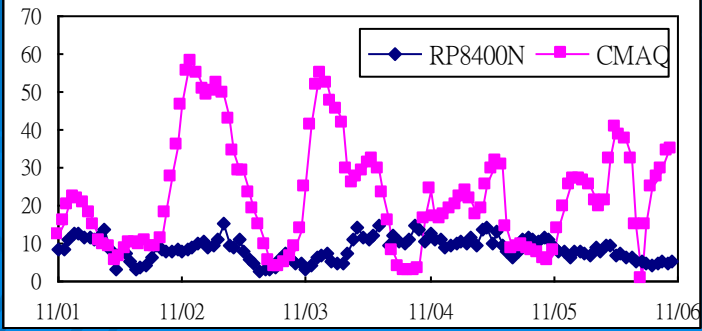
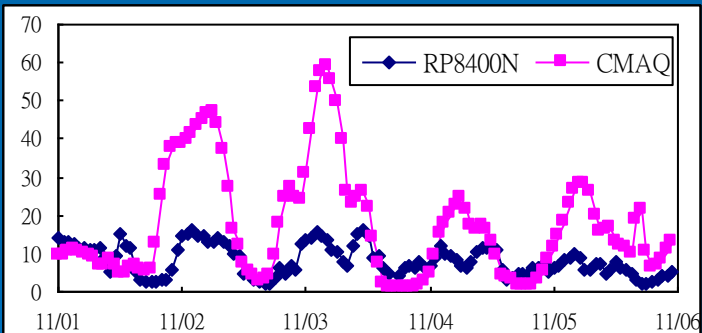
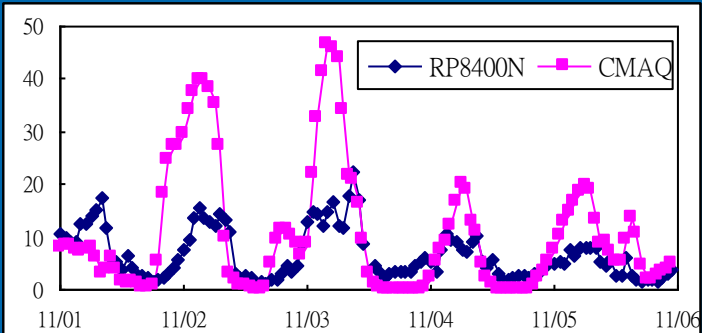
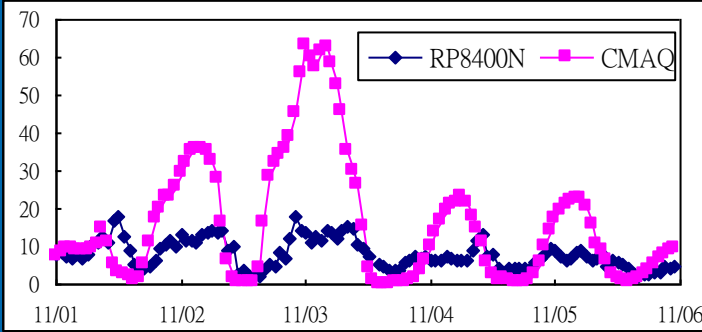


Heterogeneous HONO formation mechanism
(Ammann et al., 1998; Arens et al., 2001)

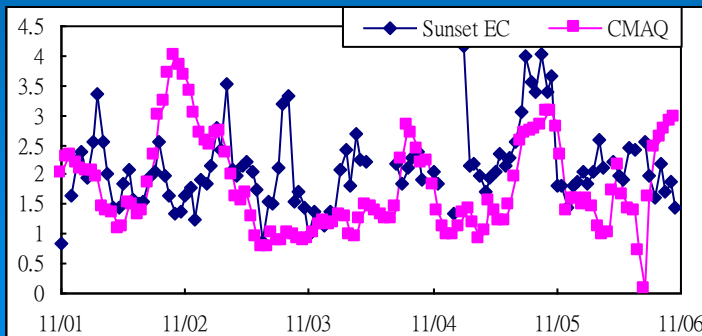
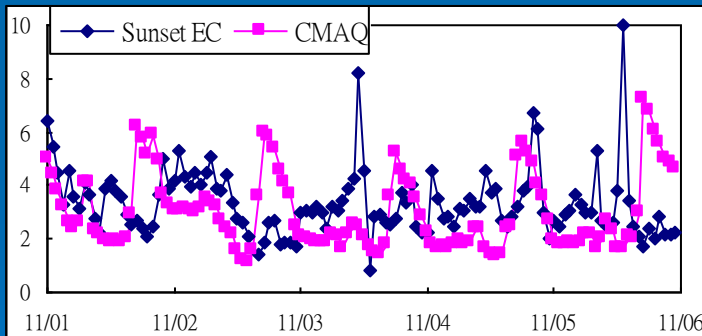
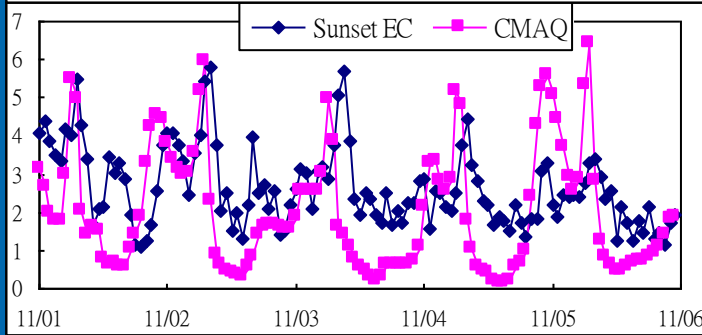
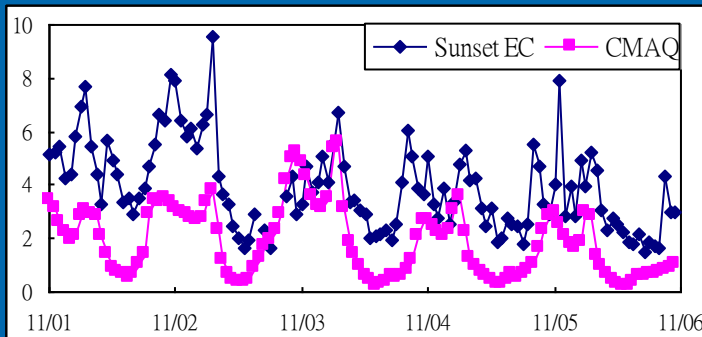
Sulfate



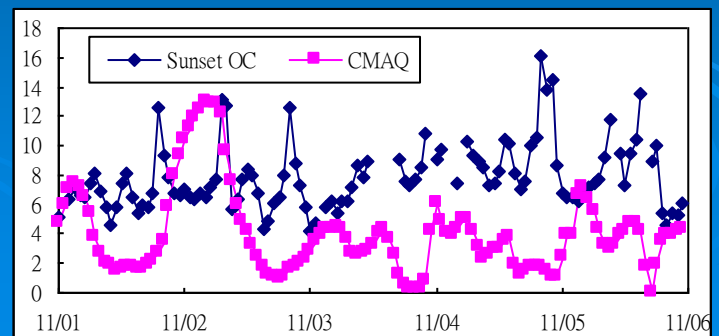
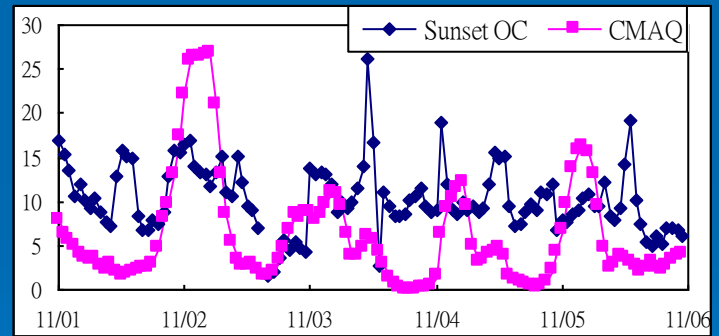
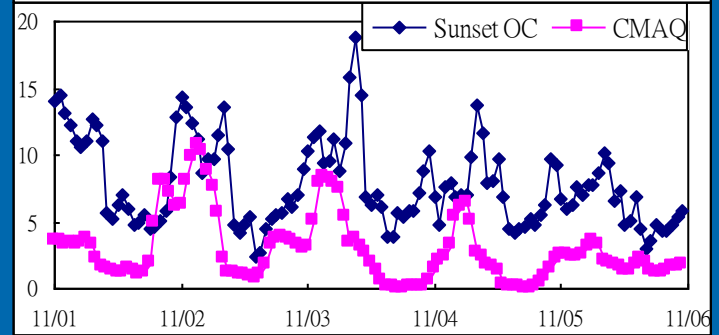
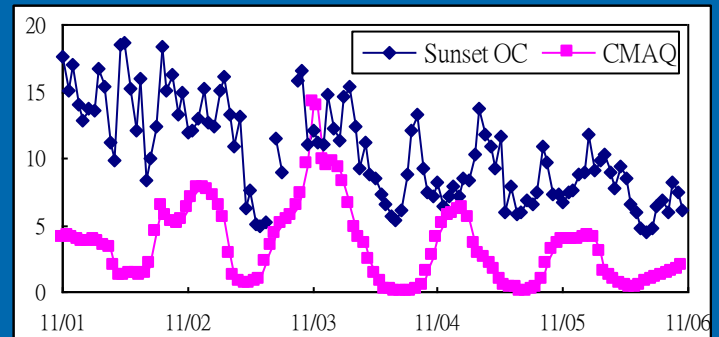
Nitrate

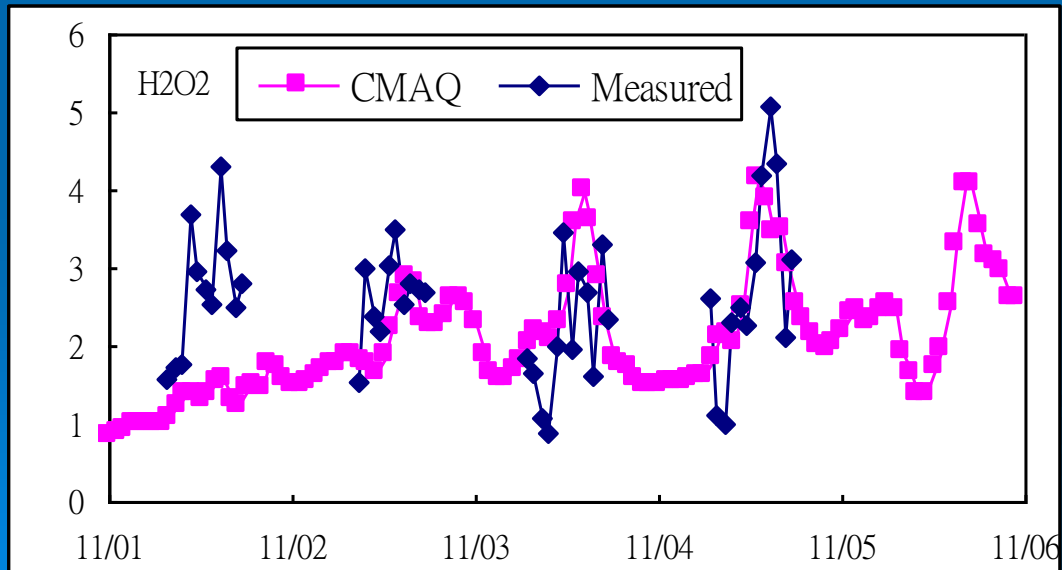
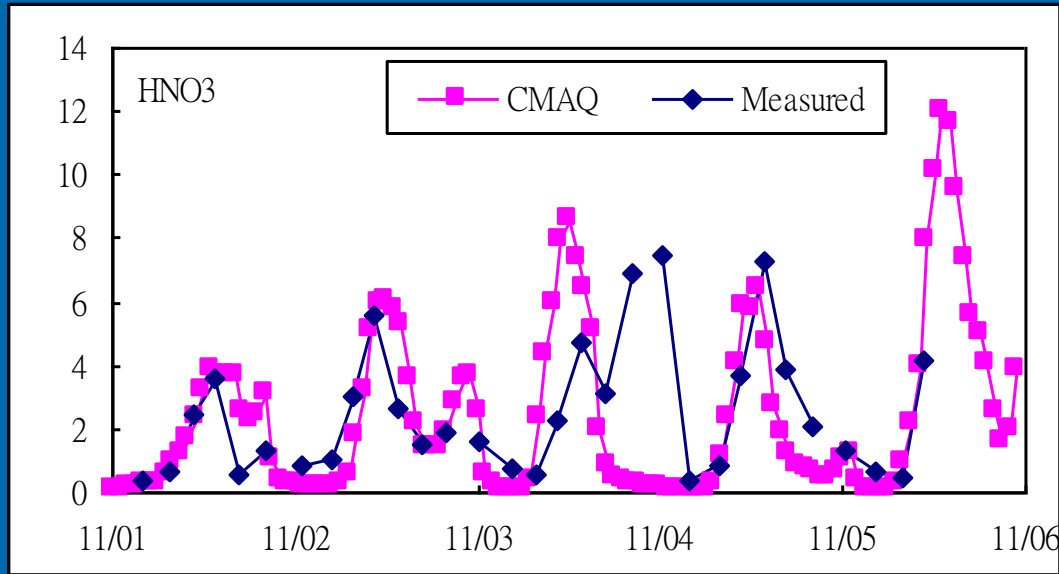


EC



OC





Ratios of Simulated to Measured

	North	West	Center	South
SO _x	2.6±1.5	1.9±1.5	2.9±3.2	2.9±2.4
NO _x	0.76±0.49	1.2±0.89	2.6±1.7	1.6±1.3
O ₃	0.92±0.38	0.61±0.25	0.53±0.34	0.55±0.35
PM	0.83±0.59	0.86±0.60	1.3±0.81	1.4±1.5
EC	0.46±0.30	0.78±0.61	1.0±0.70	0.95±0.51
OC	0.31±0.26	0.36±0.30	0.63±0.54	0.56±0.44
Nitrate	1.7±1.4	1.5±1.6	2.2±1.9	3.0±2.2
Sulfate	0.23±0.11	0.15±0.11	0.33±0.19	

Formation of Secondary PM:

Sulfate PM formation:



Gas Phase: O_2, H_2O_2



Aqueous Phase: H_2O



Nitrate PM formation:



Gas Phase : (daytime)



Gas & Aq Phase : (nighttime)



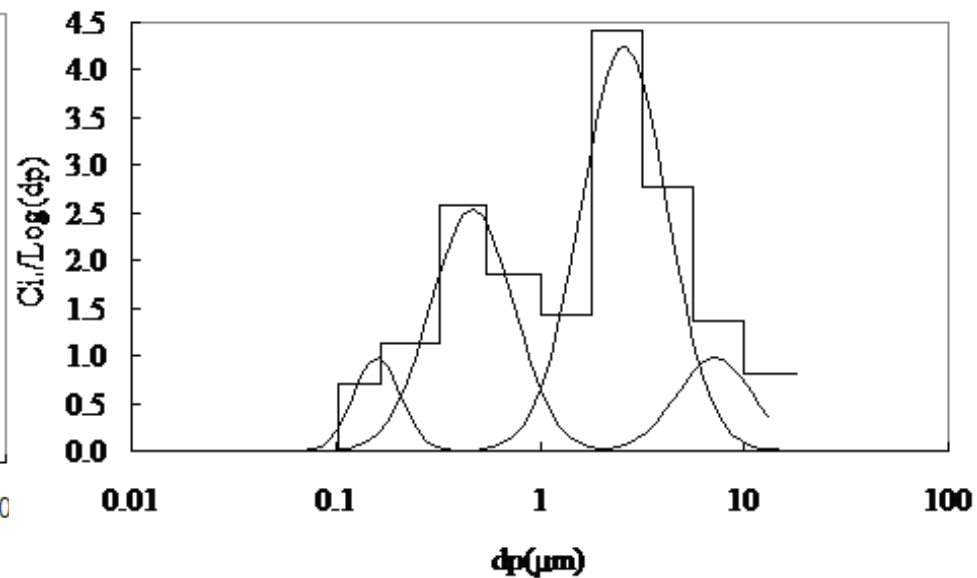
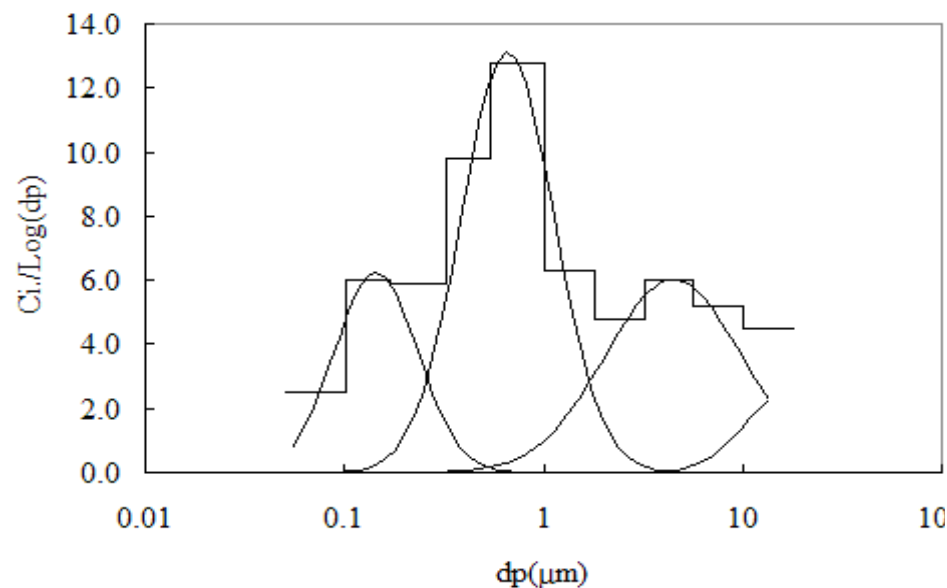
Organic PM formation:

(Gas-Particle conversion)



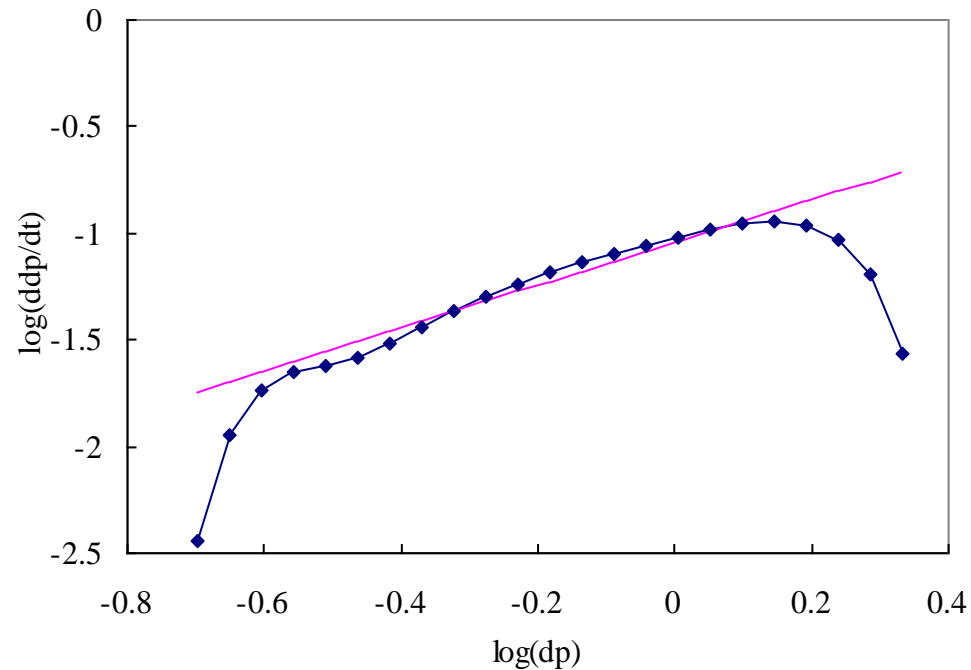
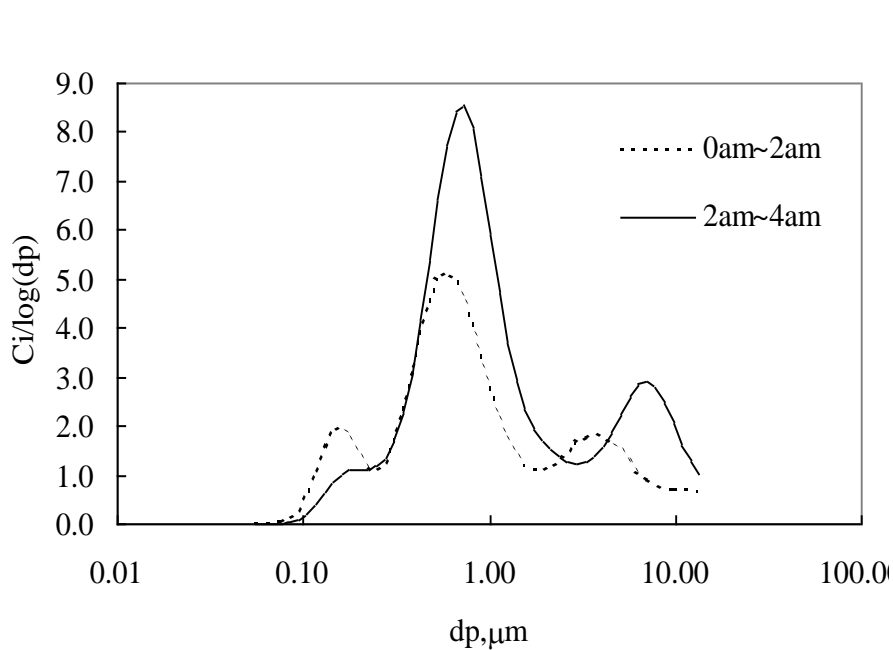
(Long-chain VOC, Aromatics, Biogenic VOC)

Size Distributions of Nitrate and Sulfate



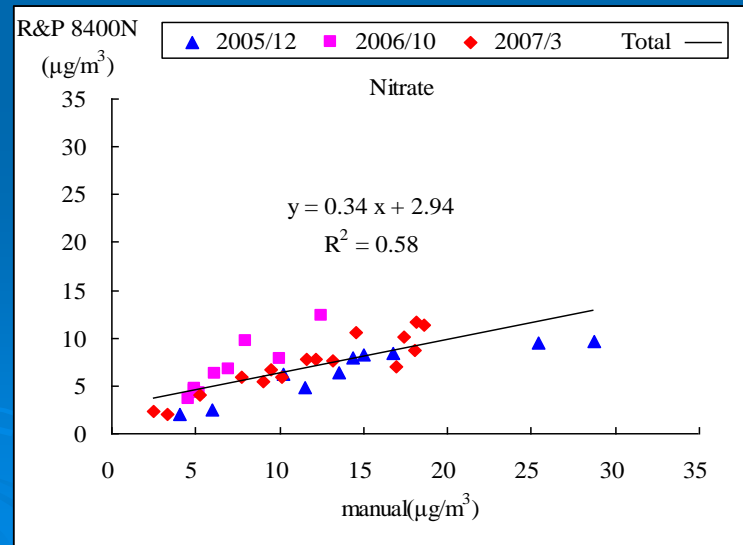
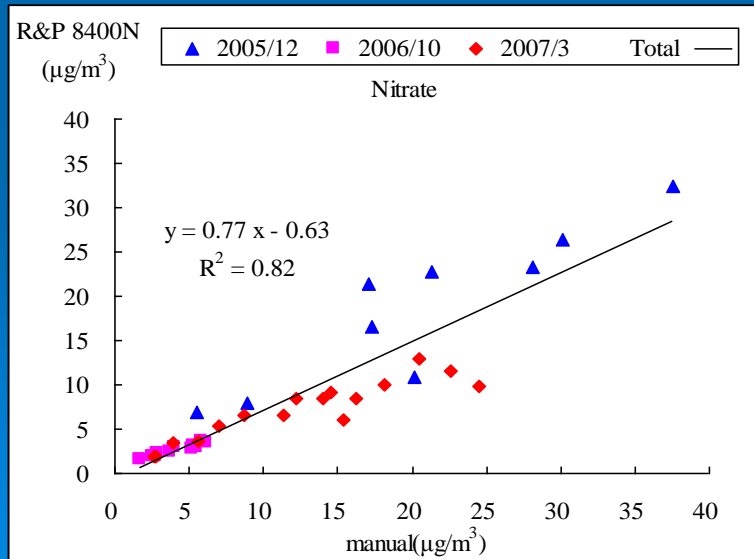
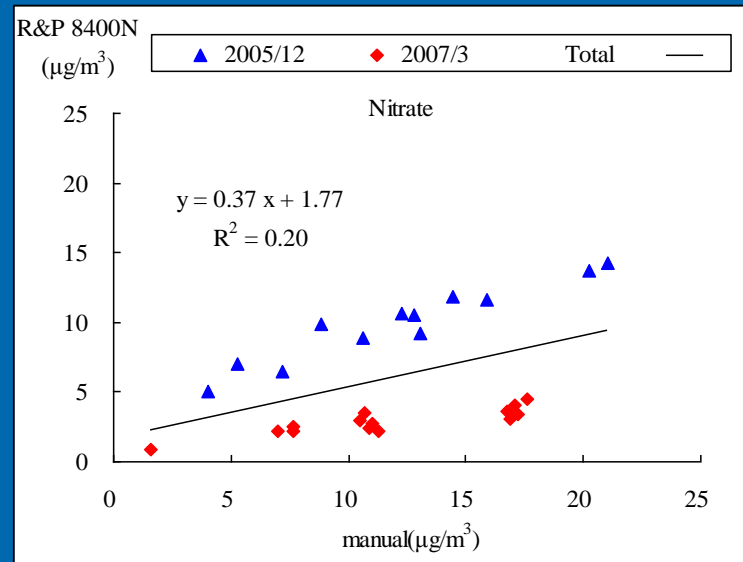
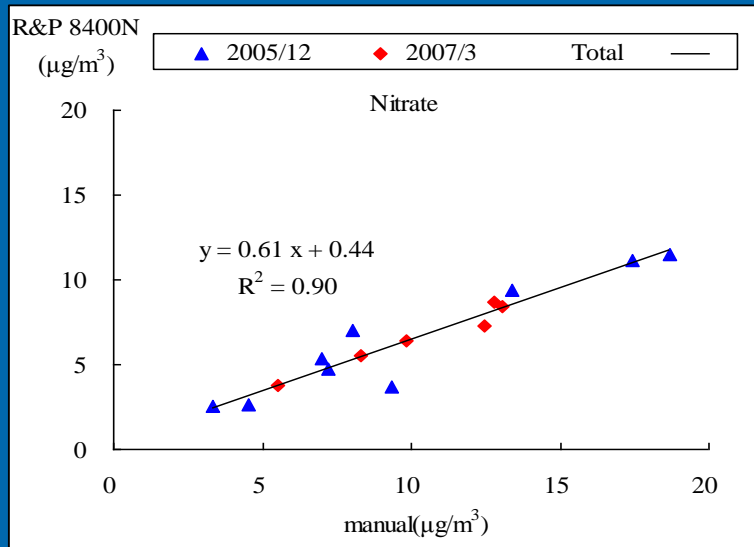
Nitrate		Sulfate	
Mode Diameter	Contribution Fraction	Mode Diameter	Contribution Fraction
0.11 to 0.14 (0.12)	13.8 to 45.2 (22.2)	0.11 to 0.12 (0.12)	15.0 to 23.7 (14.3)
0.33 to 0.74 (0.51)	21.8 to 54.8 (41.9)	0.37 to 0.58 (0.47)	30.4 to 58.8 (36.3)
4.27 to 6.00 (4.80)	29.1 to 46.8 (36.2)	1.22 to 1.49 (1.36)	29.3 to 45.9 (28.1)
		3.91 to 4.61 (4.32)	25.8 to 33.5 (21.4)

Formation Mechanisms of Sulfate

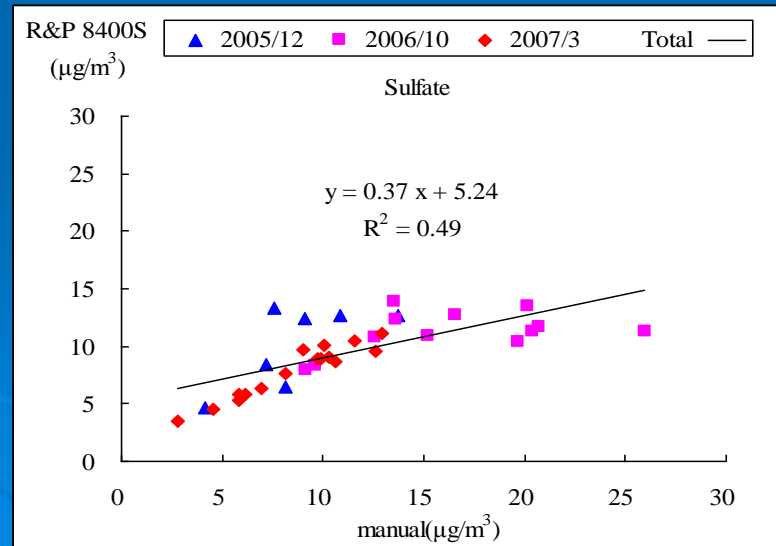
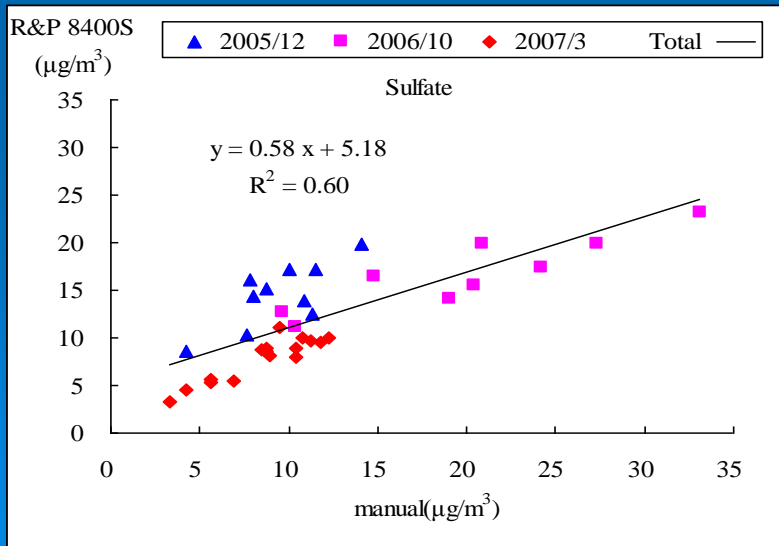
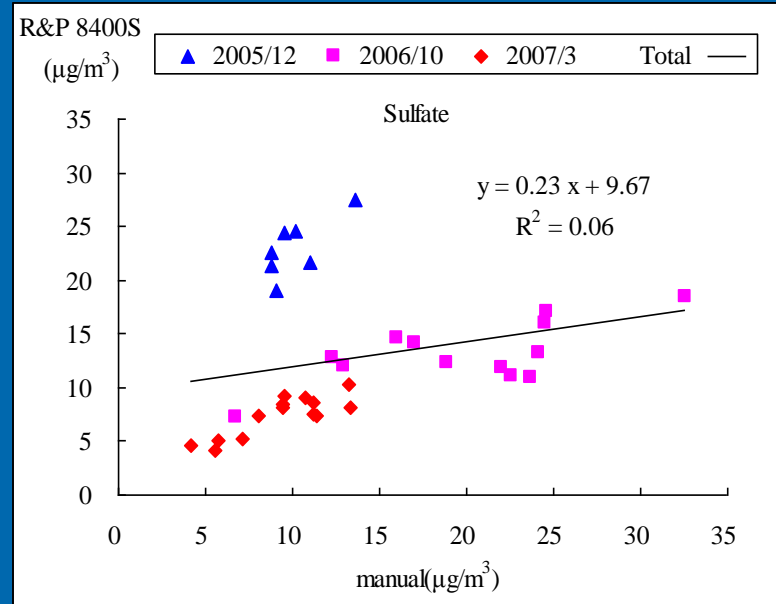
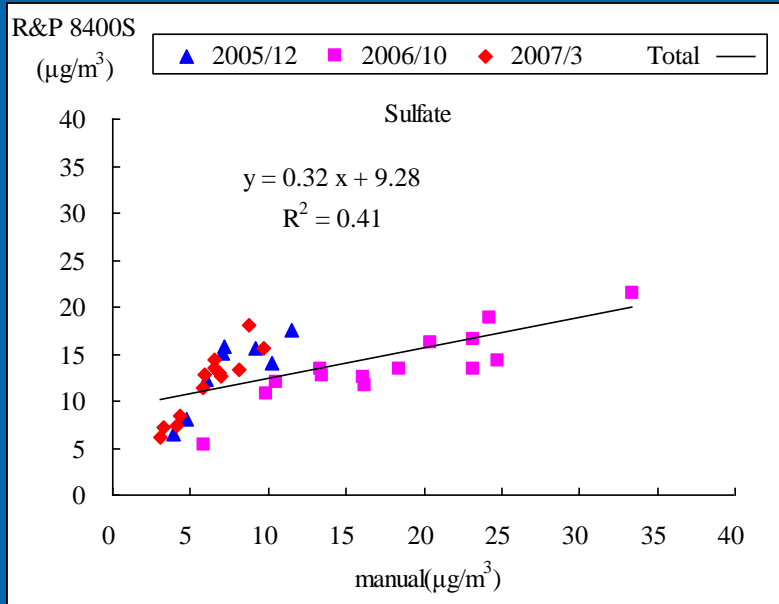


Size distributions for sulfate measured in sequences and the computed particle growth rates. The straight line is for curve with slope of one.

RP8400N vs. Denuder



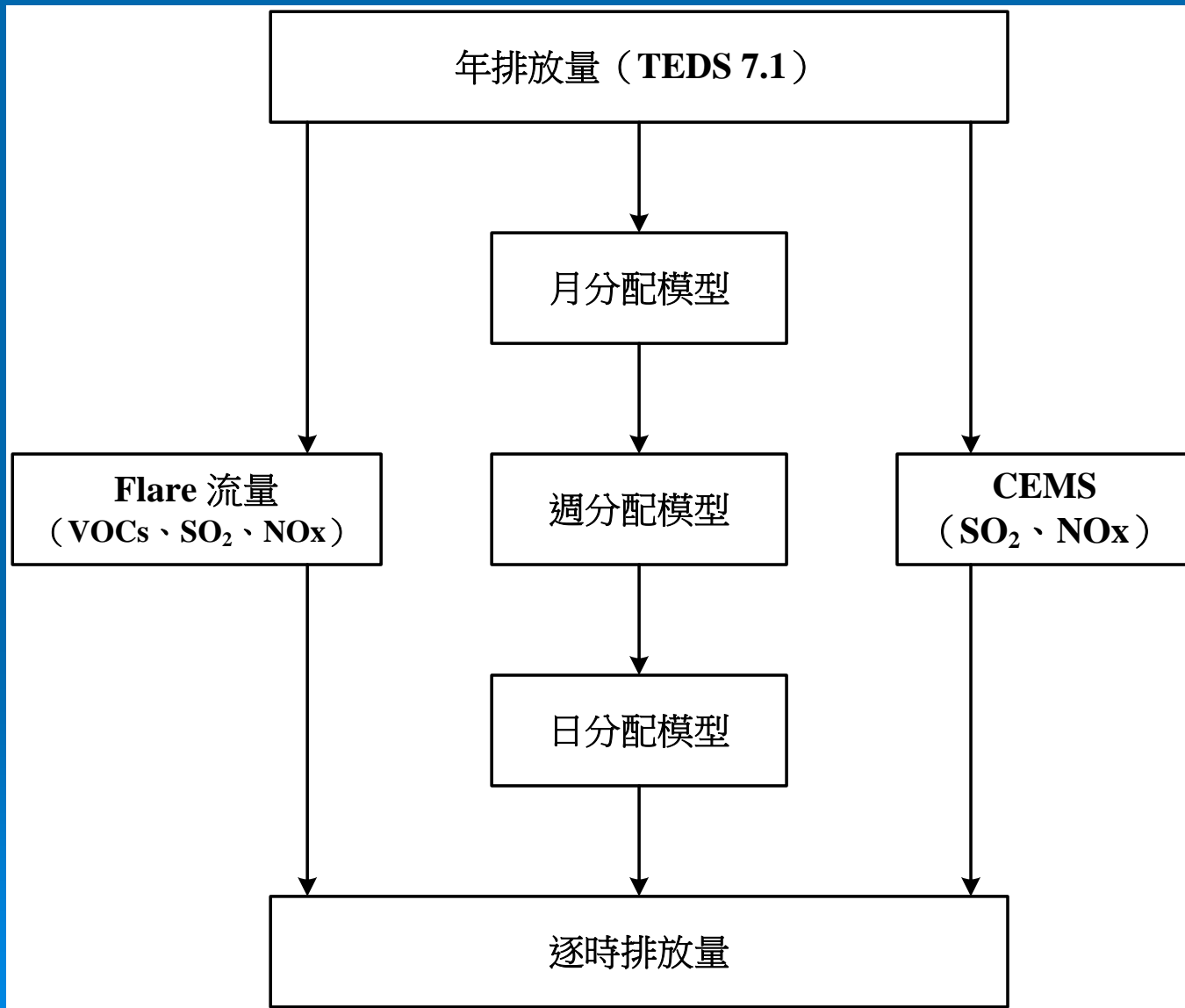
RP8400S vs. Denuder



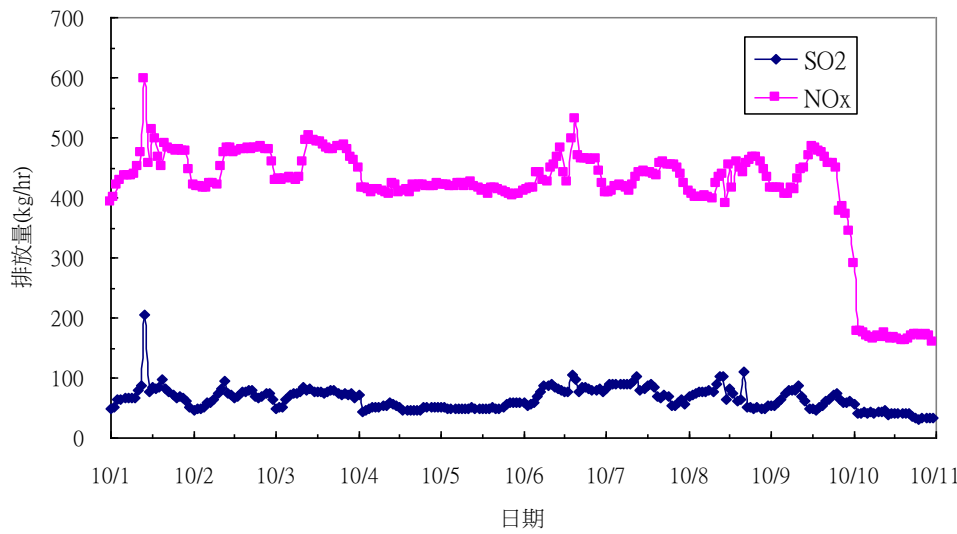
Theoretical Conversions of RP8400

Site	RP8400S		RP8400N	
	Na_2SO_4	$(\text{NH}_4)_2\text{SO}_4$	KNO_3	NH_4NO_3
North	49	23	88	72
West	62	20	84	67
Center	64	31	90	83
South	67	28	84	76

建置逐時排放量

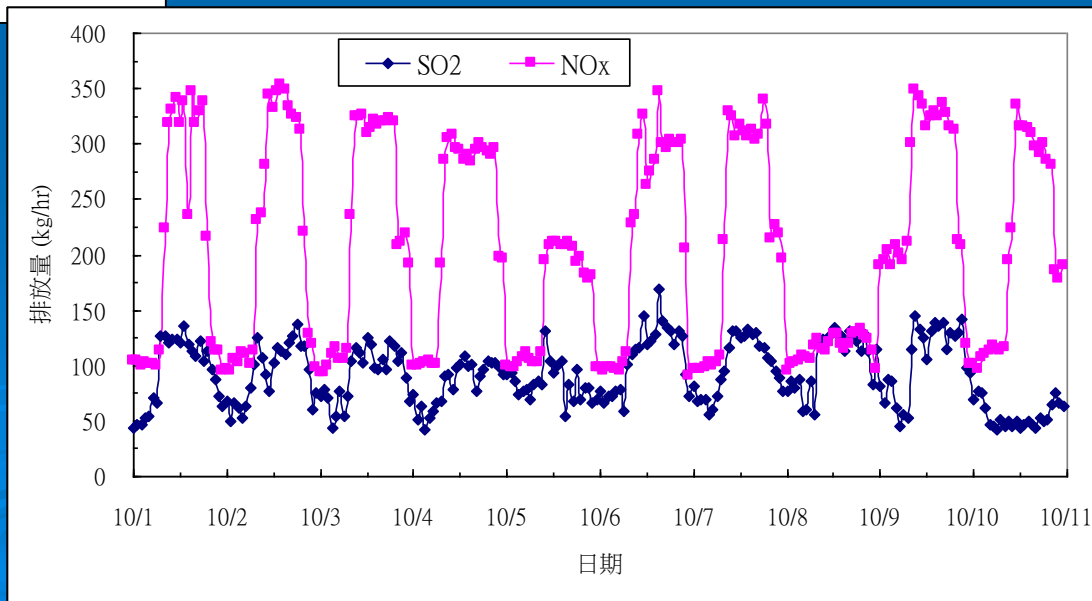


嘉義縣與台南縣CEMS之逐時排放量

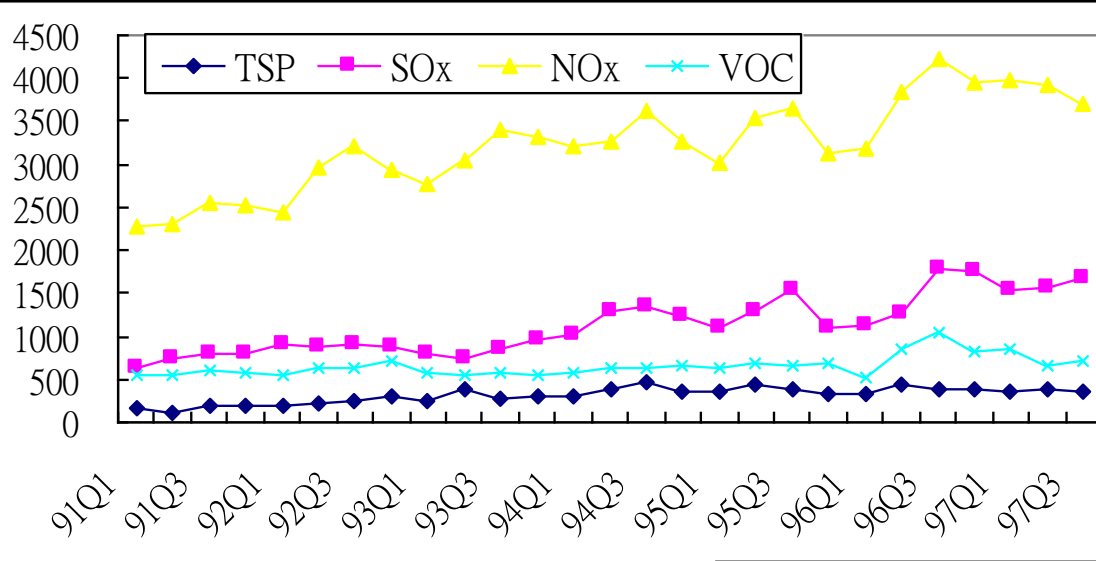


台南縣

嘉義縣

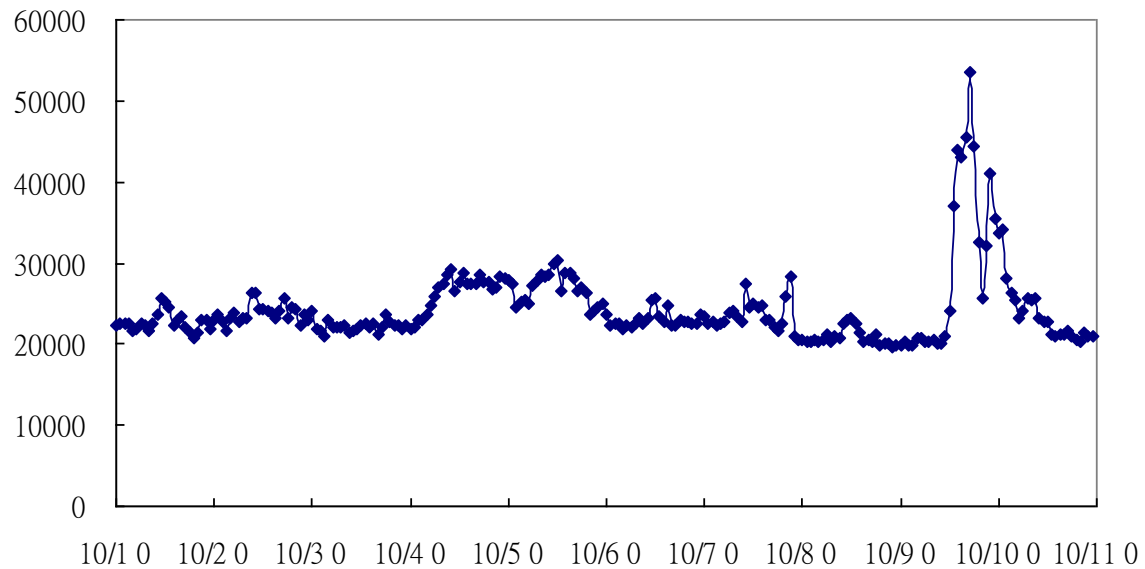


離島工業區



廢氣燃燒塔逐時
流量(Nm³/hr)

逐季網路申報
排放量(公噸)




Summary

- Ozone concentrations have been simulated by CMAQ fairly;
- The error of simulated PM mass is generally within a factor of two;
- Fair agreements for nitrate and EC;
- Both sulfate and OC are underestimated.

*Conversion of S(IV) to S(VI)
in aerosol water*

Suggestions

- **Formation of sulfate in aerosol water should be included;**
 - **Better measurement methods for hourly species concentrations should be developed;**
 - **Temporal variations of hourly emission profiles should be developed.**
- 

*Thanks for Your
Attentions.*

