Model Development to Investigate Boundary layer processes and Air Quality

Xiao-Ming Hu

Center for Analysis and Prediction of Storms, School of Meteorology

University of Oklahoma

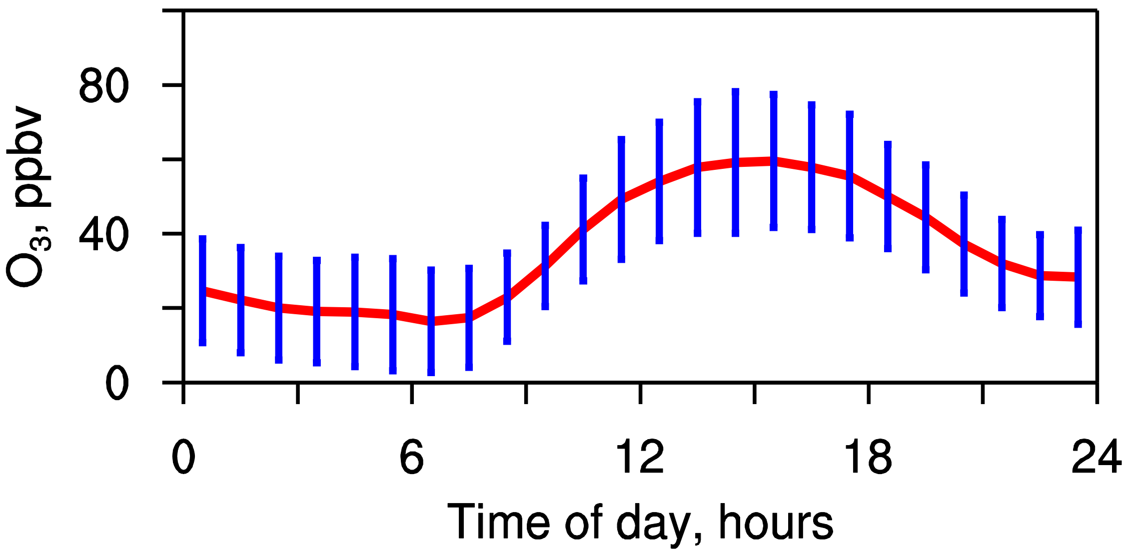
June 2, 2017

Guangzhou Institute of Geochemistry

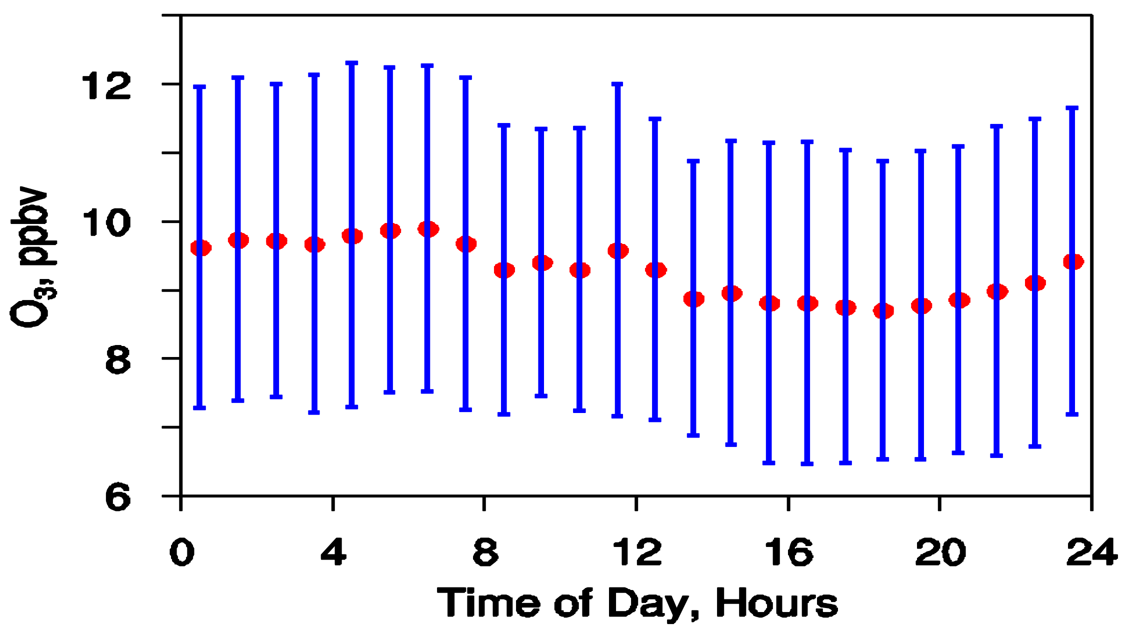
Chinese Academy of Sciences

1. **0D gas phase mechanism model**
   to simulate O_3 over ocean
2. **1D chemistry model**
   to simulate impact of boundary layer processes
3. **Slab dispersion model**
   to investigate air quality in the NCP
4. **SREF-WRF/Chem ensemble system**
   to investigate air quality in Dallas

Unique O_3 diurnal variation over Ocean



Continental BL with
~10 ppbv NO_x
(Hu et al., 2012)



Marine BL with
~10 pptv NO_x
(Hu et al., 2010)

Ozone production and destruction

Production:

$$NO_2 + h\nu \rightarrow NO + O(^3P)$$

$$O(^3P) + O_2 + M \rightarrow O_3 + M$$

Destruction:

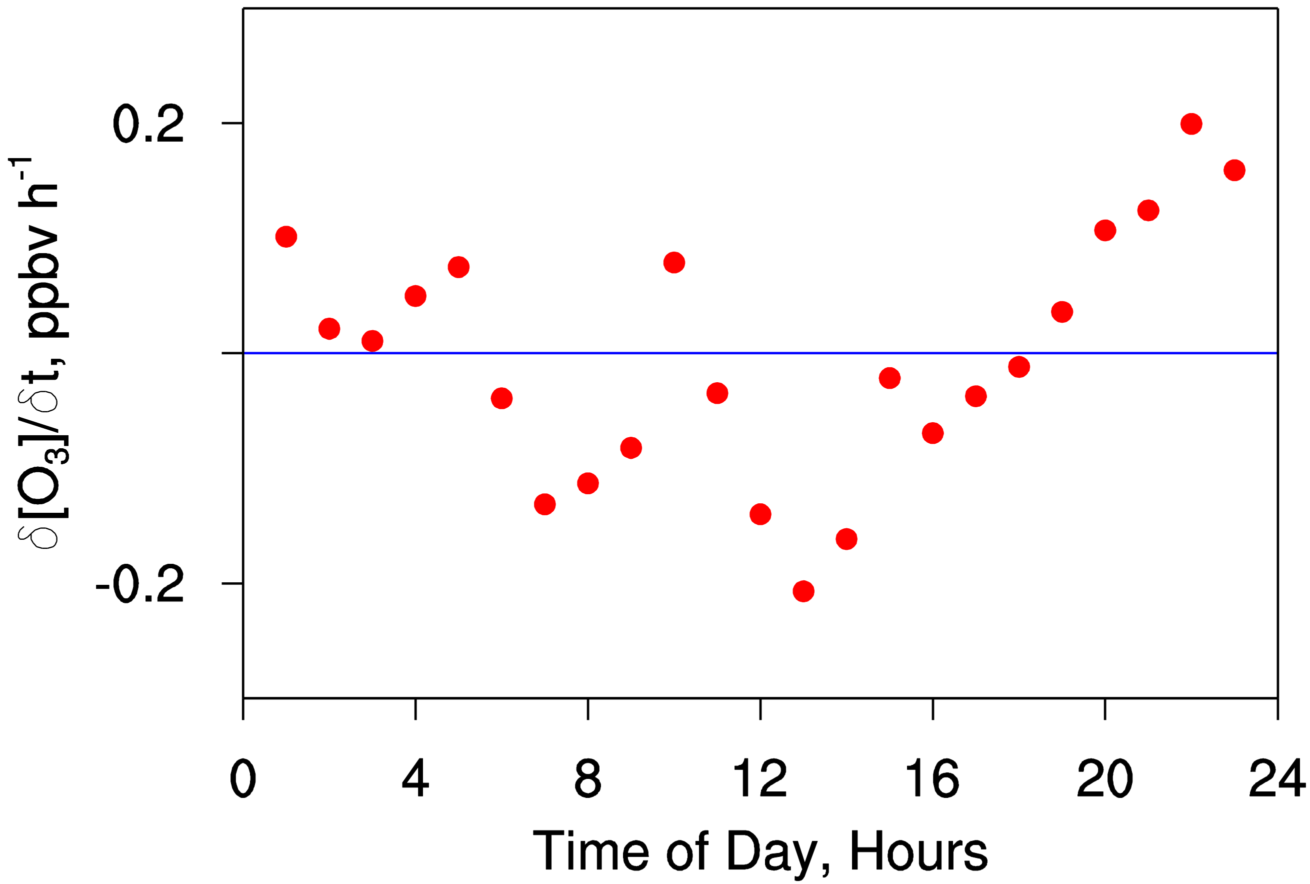
$$O_3 + h\nu \rightarrow O(^1D) + O_2$$

$$O_3 + OH \rightarrow HO_2 + O_2$$

$$O_3 + HO_2 \rightarrow OH + 2O_2$$

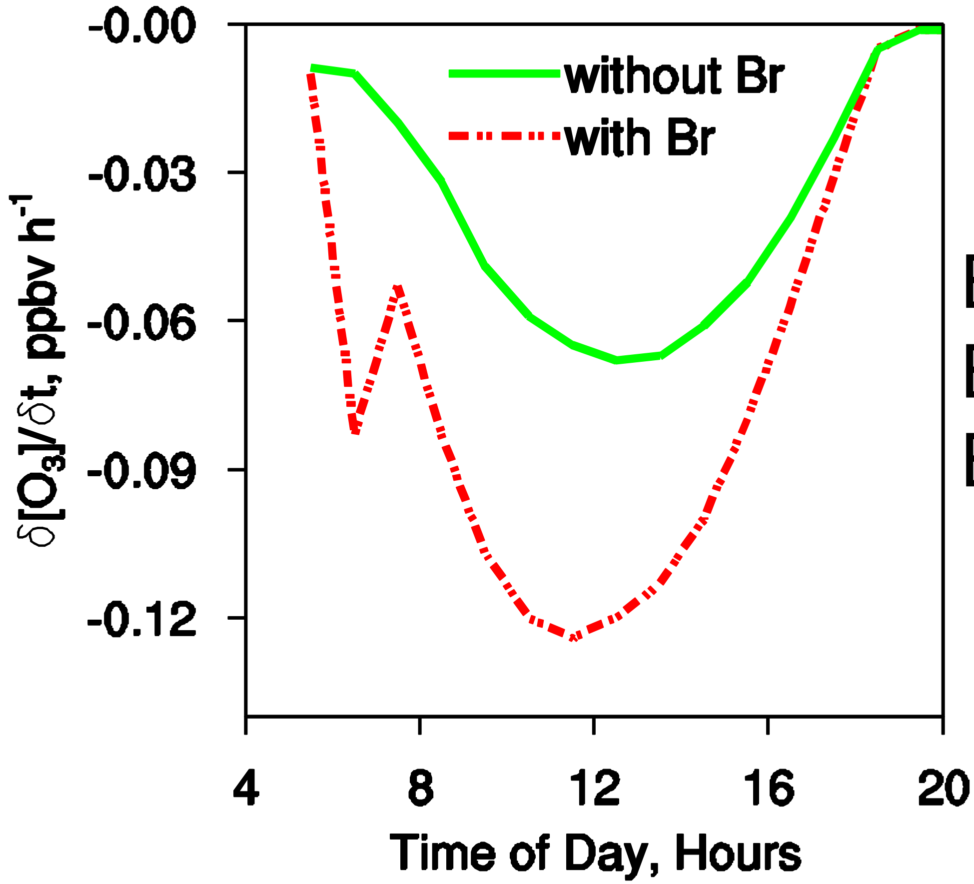
With enough NOx, O_3 production dominates; otherwise O_3 destruction dominates

Ozone destruction in the marine BL, observation



Two peaks are observed in the daytime ozone change rate ($\delta[O_3]/\delta t$) at Kwajalein

Contribution of Br chemistry to O_3 destruction, 0D simulation



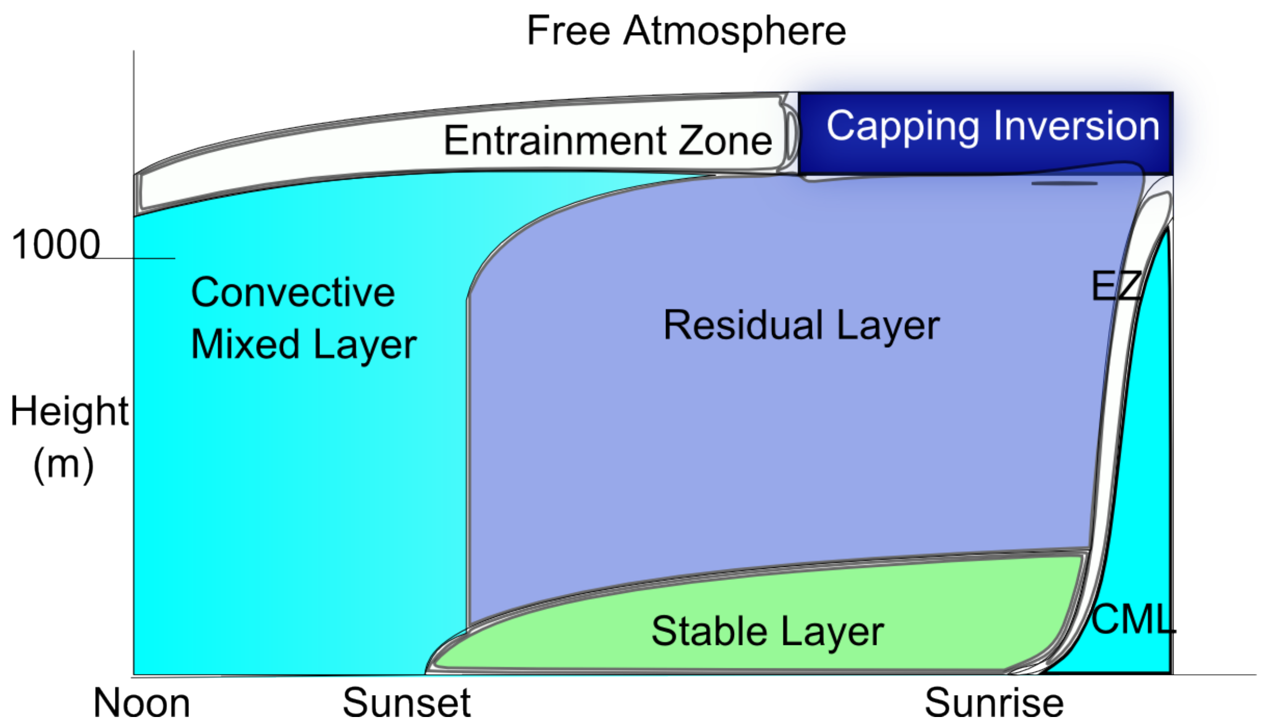
$$Br_2 + h\nu \rightarrow 2Br$$
$$Br + O_3 \rightarrow BrO + O_2$$
$$BrO + HO_2 \rightarrow HOBr + O_2$$

Br chemistry is responsible for the O_3 destruction peak in the early morning

Hu et al., 2010

1. **0D gas phase mechanism model**
   to simulate O_3 over ocean
2. **1D chemistry model**
   to simulate impact of boundary layer processes LLJs in the eastern US urban corridor
3. **Slab dispersion model**
   to investigate air quality in the NCP
4. **SREF-WRF/Chem ensemble system**
   to investigate air quality in Dallas

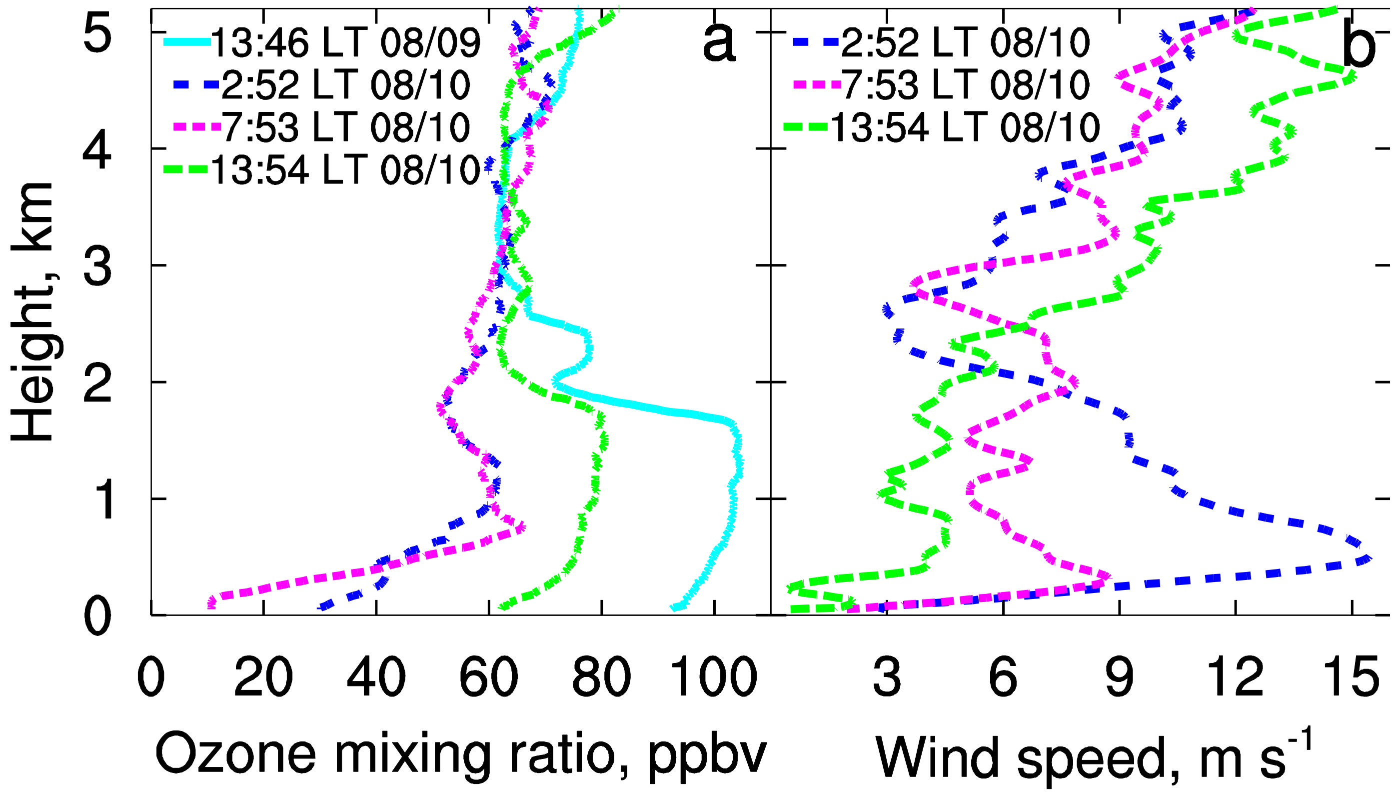
Impact of LLJs on BL O_3, Classical view of the residual layer



Modified from Stull

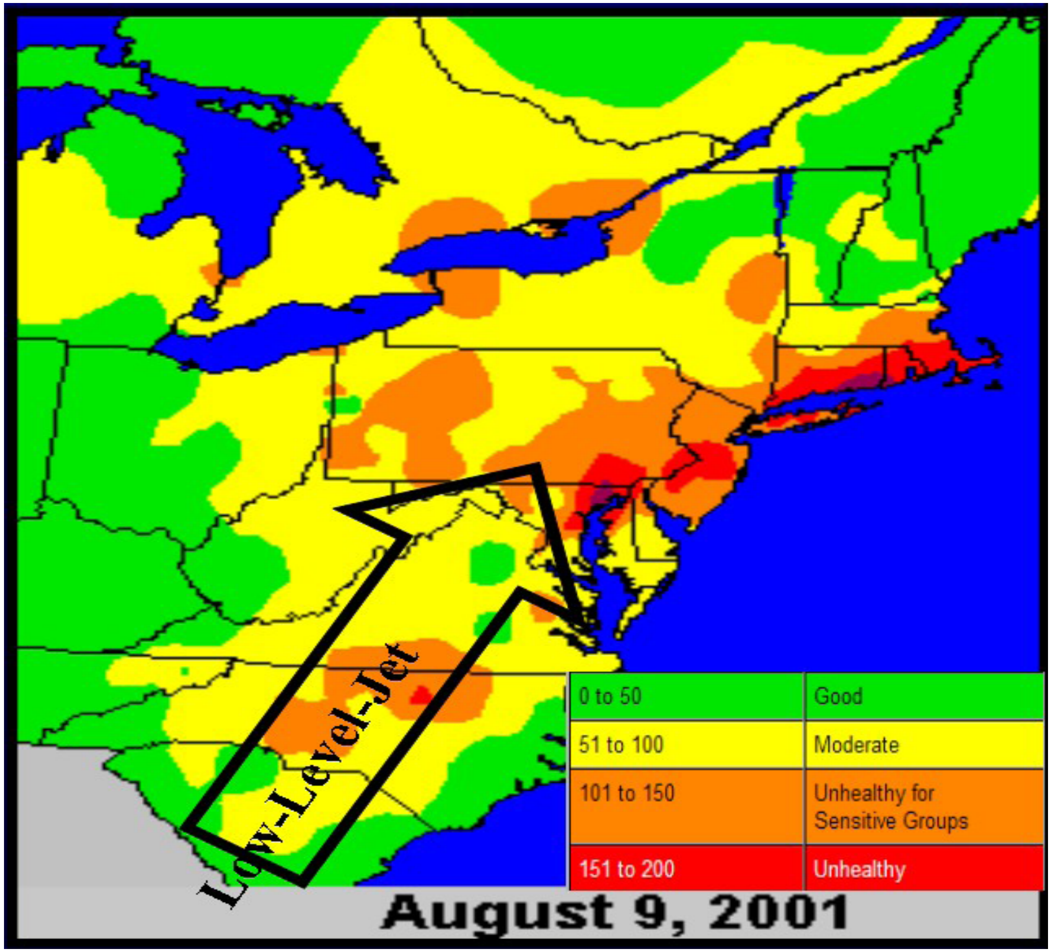
The residual layer is often thought to be a reservoir of pollutants

Observation challenges the classical view of the residual layer



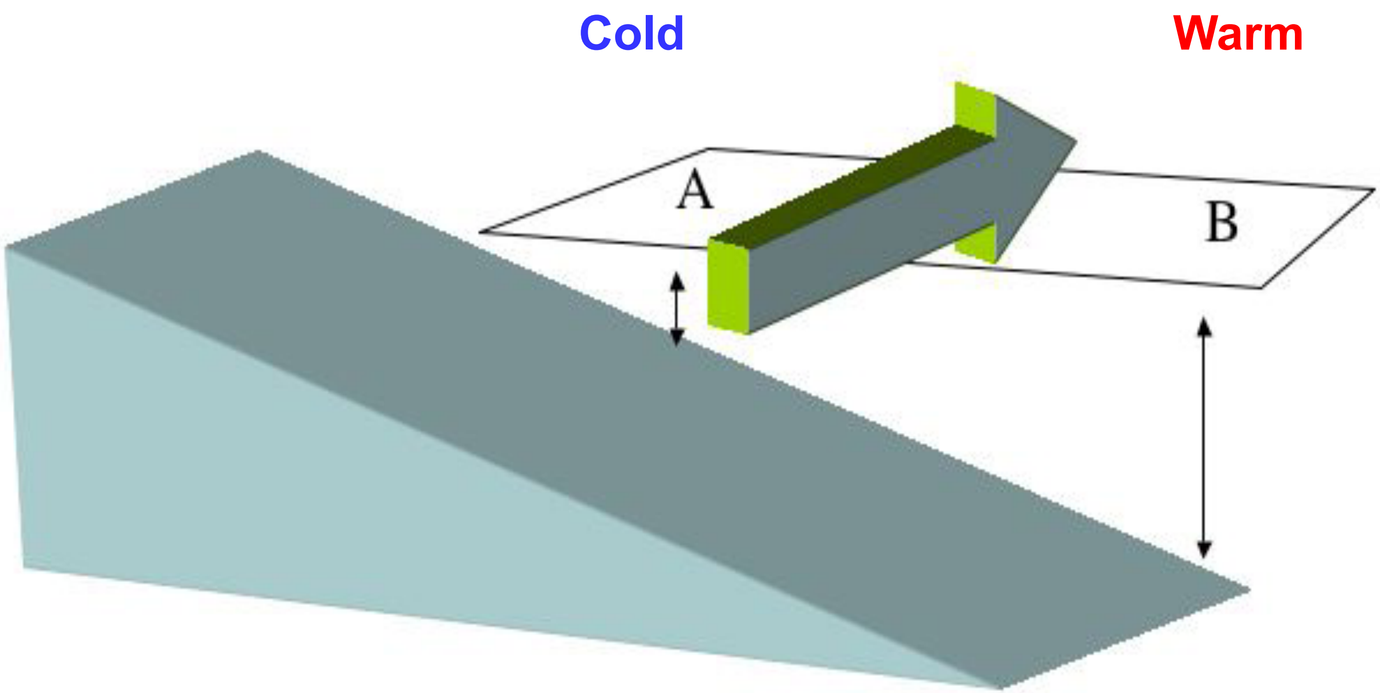
The residual layer in Beltsville is rarely a reservoir of O_3 (Hu et al., 2013)

Mid-Atlantic costal LLJs



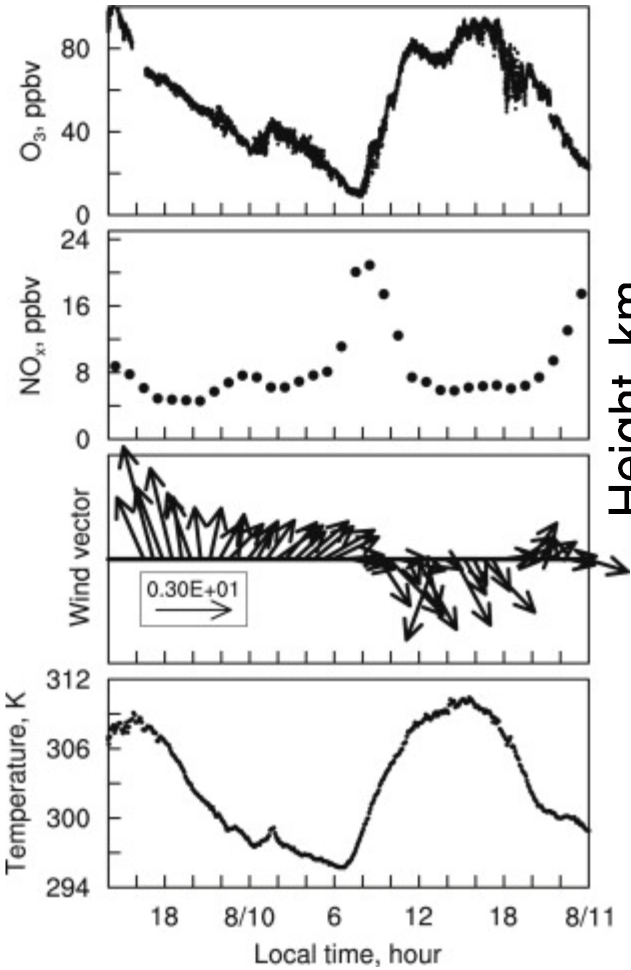
LLJs occur frequently in the eastern costal area. (Figure: Air quality index during an ozone episode, Ryan and Piety, 2001)

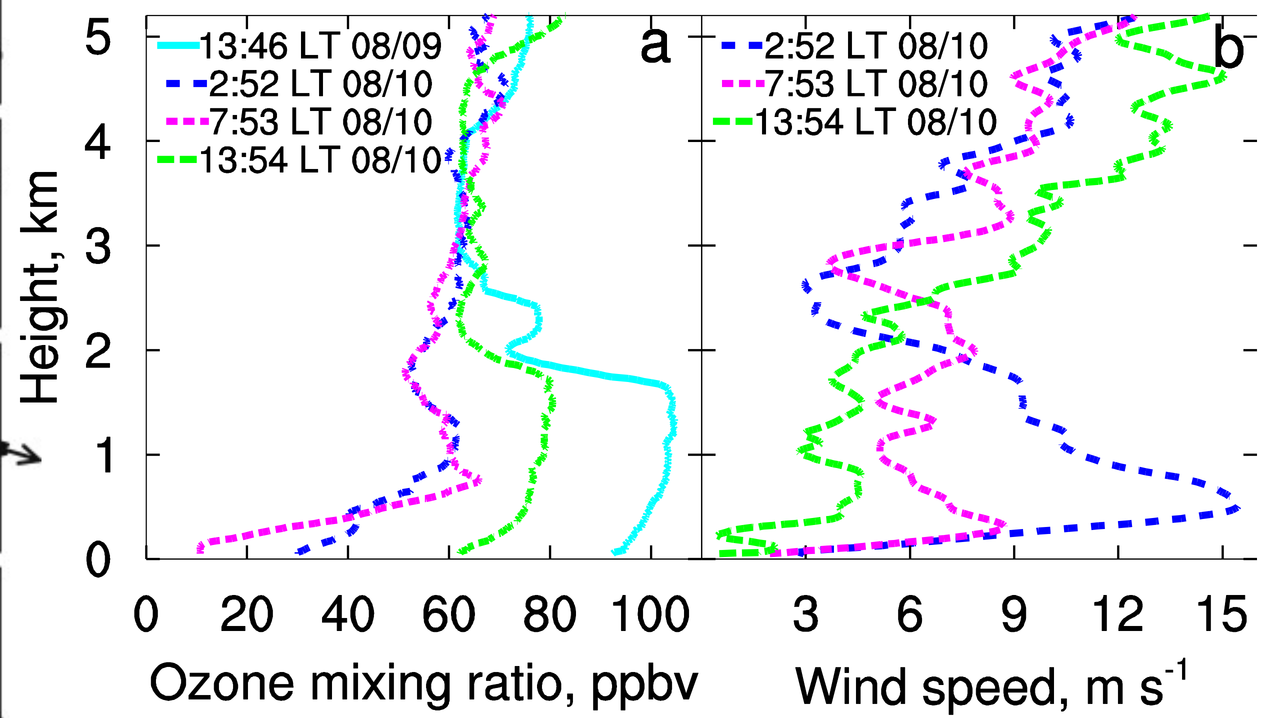
LLJs formation in Beltsville



Thermal wind contributed to the formation of the Mid-Atlantic costal LLJs

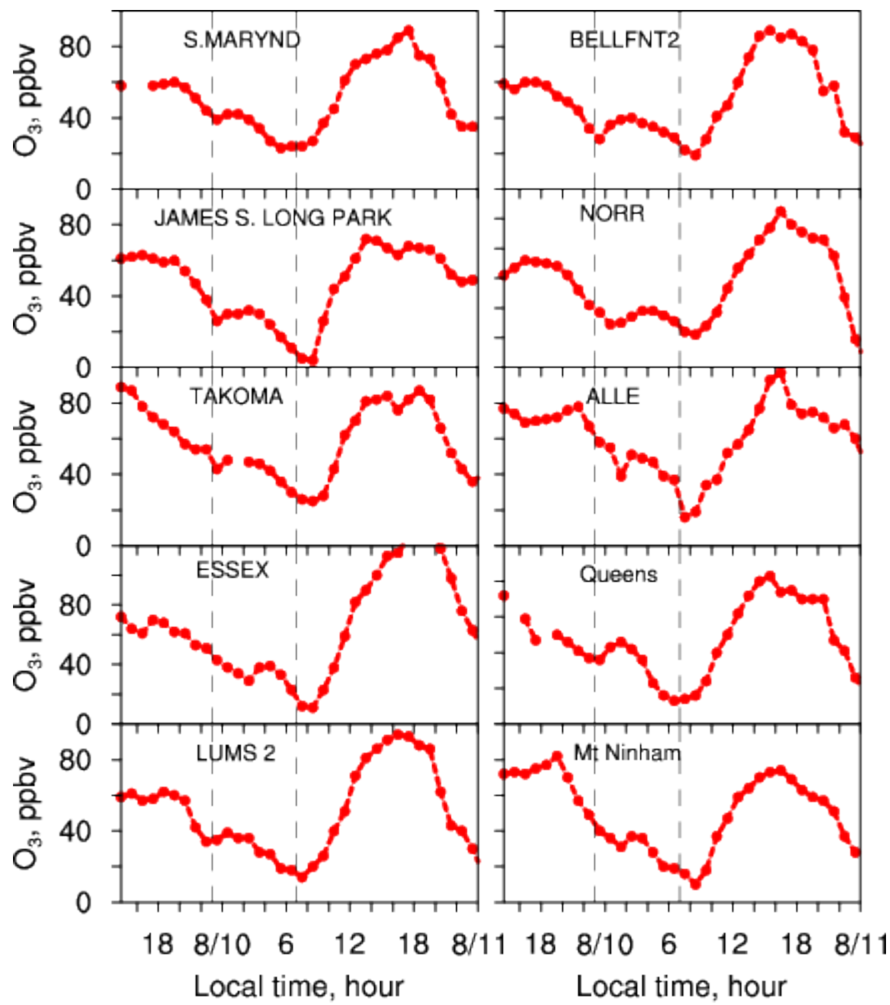
Case study of August 10, 2010, Observation



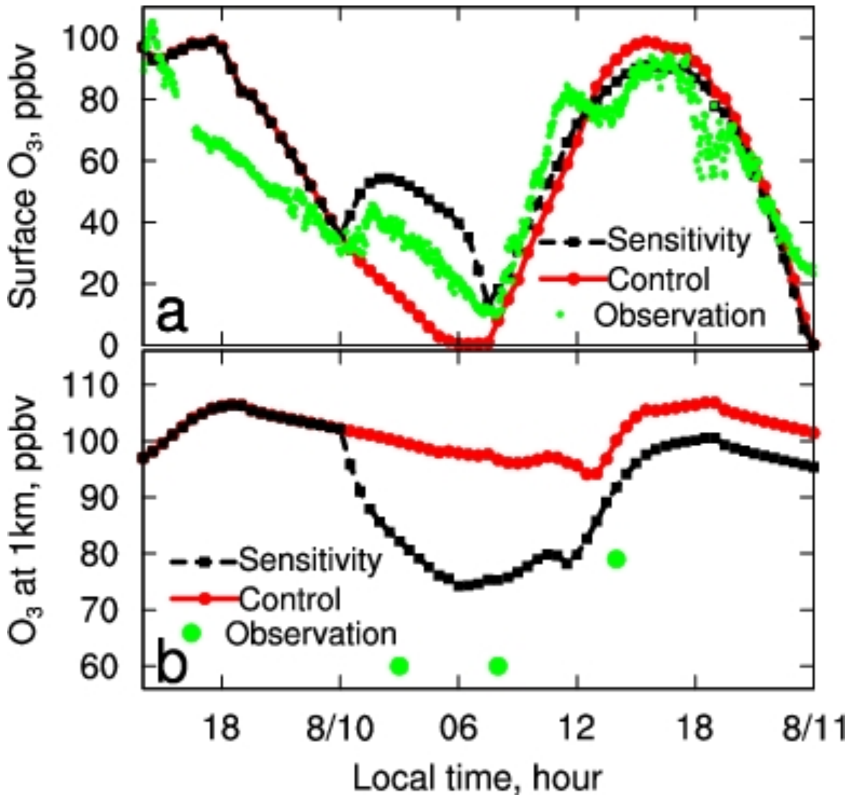


It appears a LLJ played an important role in vertical O_3 redistribution (Hu et al., 2013)

Nocturnal O_3 maxima



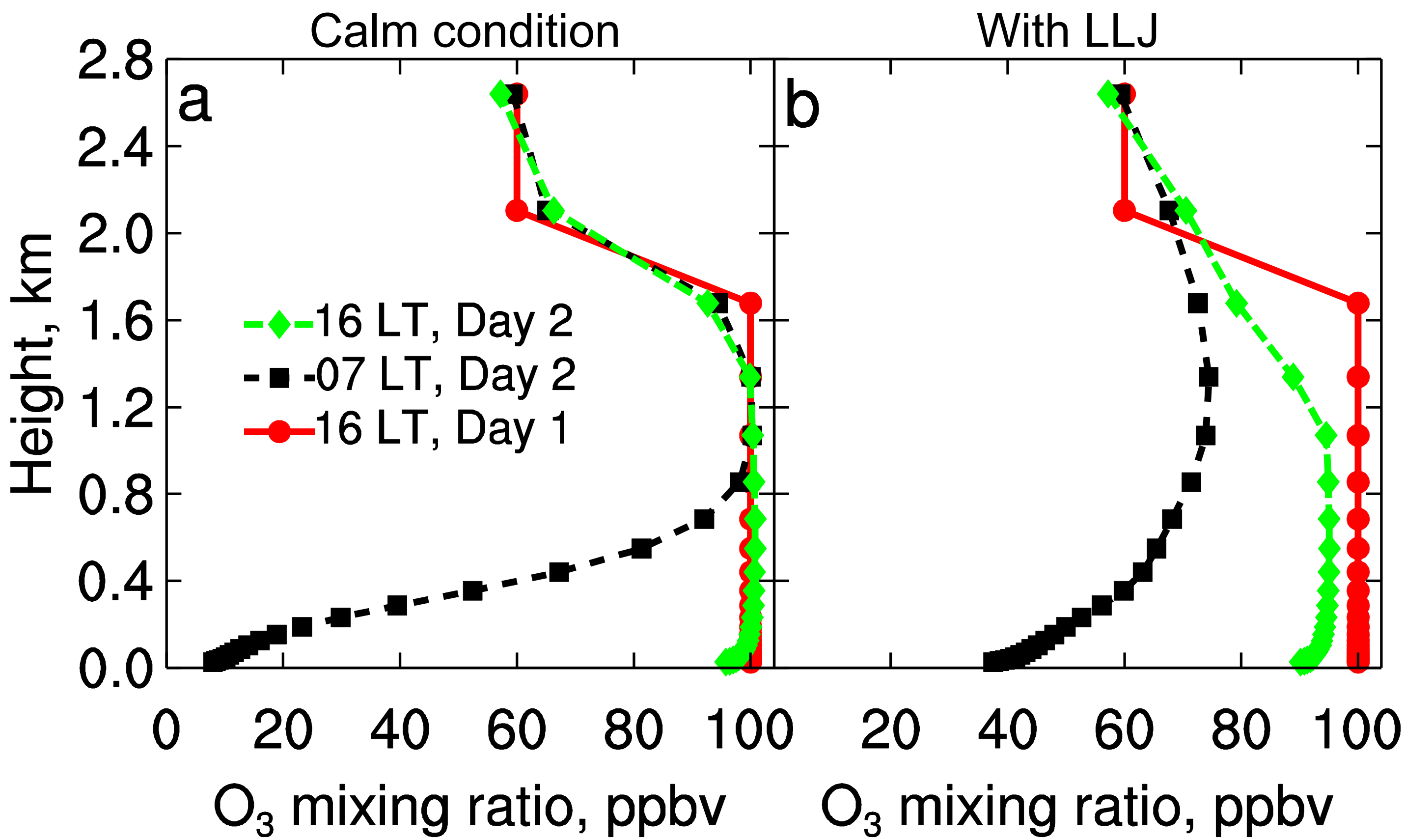
Case study of August 10, 2010, 1D simulations



Control : Calm condition, no LLJ
Sensitivity: with LLJ

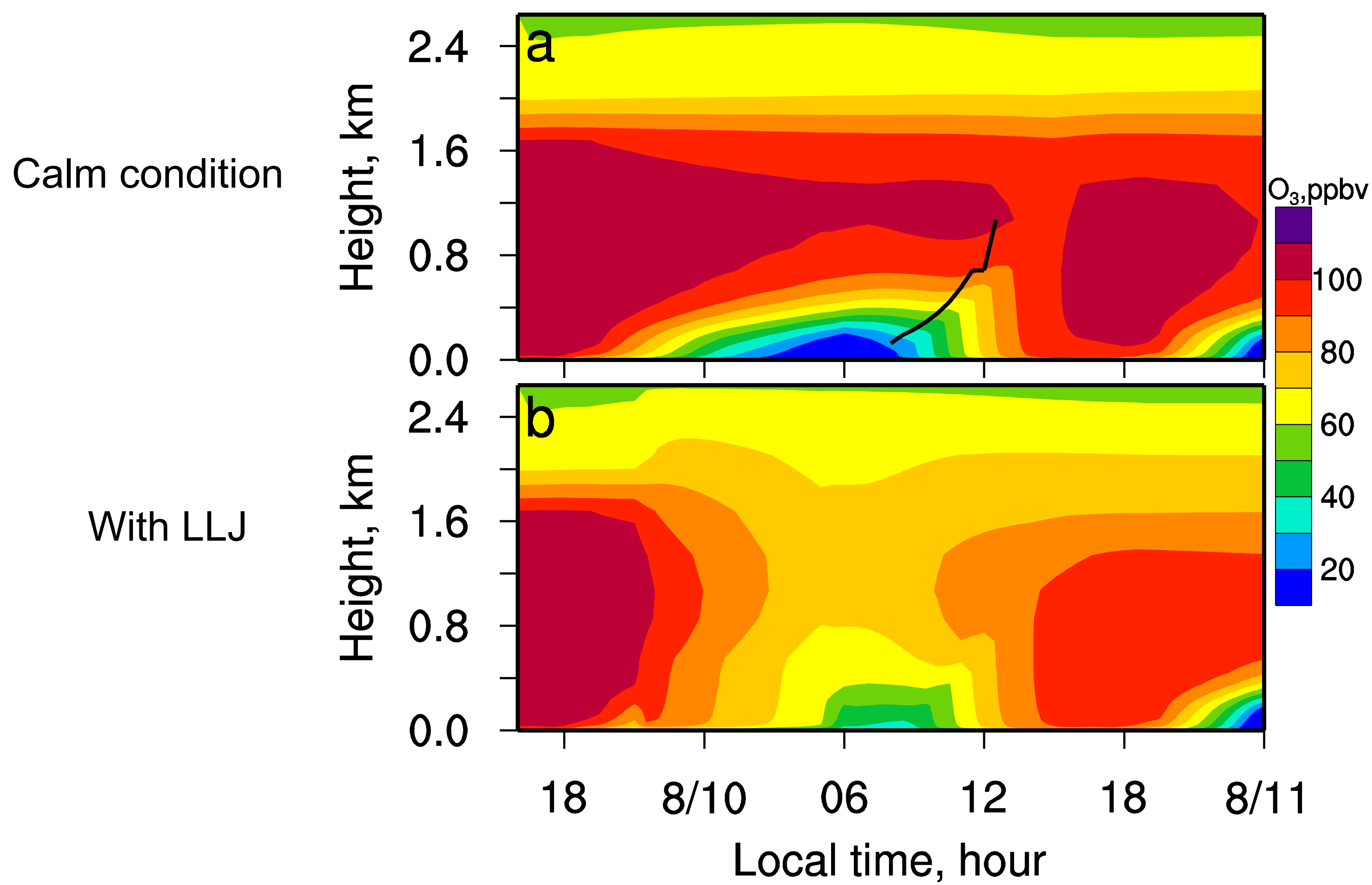
Simulation could capture the main features associated with the LLJ.

Simulated profiles of O_3 w/o & with LLJ



The presence of the LLJ reduces the RL O_3 substantially. Downward transported O_3 is removed near the surface by dry deposition and chemistry reactions. As a result the BL O_3 on the following day is reduced.

Time-height diagrams of simulated O_3



The RL is not a reservoir of O_3 in the presence of a strong LLJ

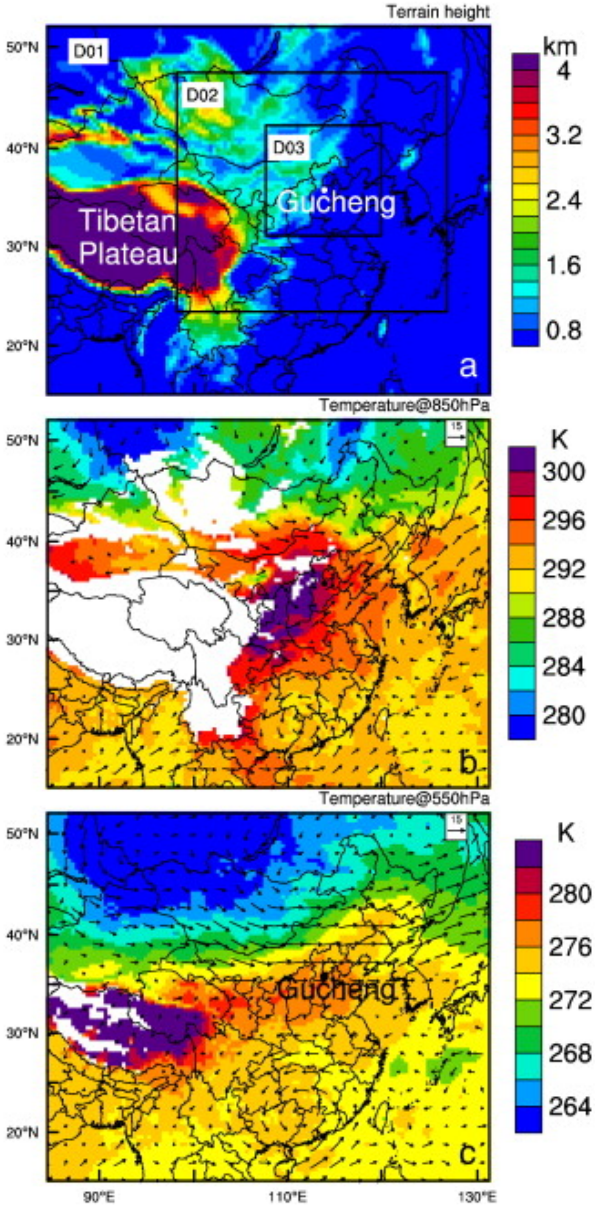
1. **0D gas phase mechanism model**
   to simulate O_3 over ocean
2. **1D chemistry model**
   to simulate impact of boundary layer processes
3. **Slab dispersion model**
   to investigate air quality in the NCP
4. **SREF-WRF/Chem ensemble system**
   to investigate air quality in Dallas

North China Plain, heat source

Terrain height

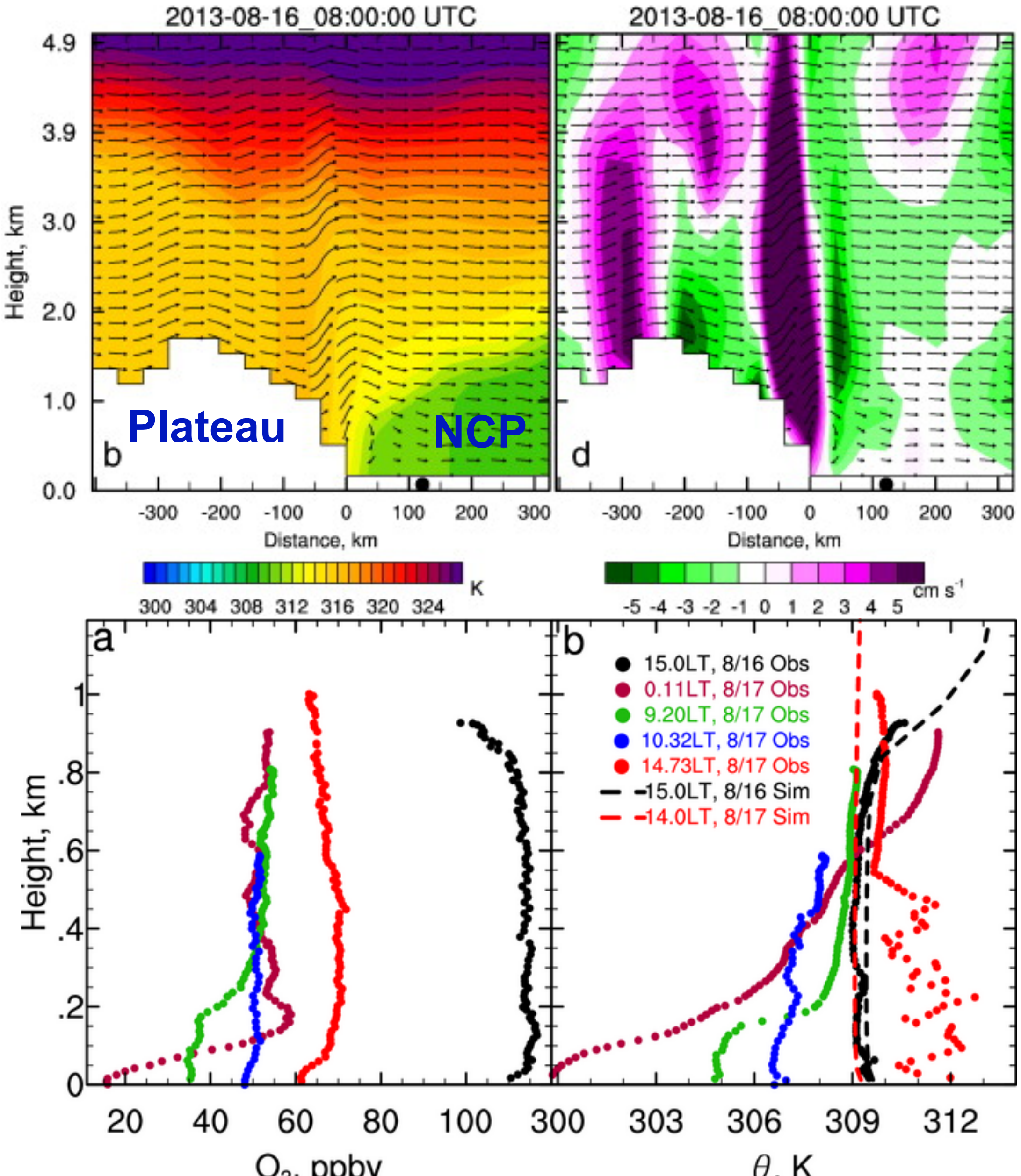
T@850hPa

T@550hPa



The Plateau acts as a heated source in Summer (Hu et al., 2014, STE)

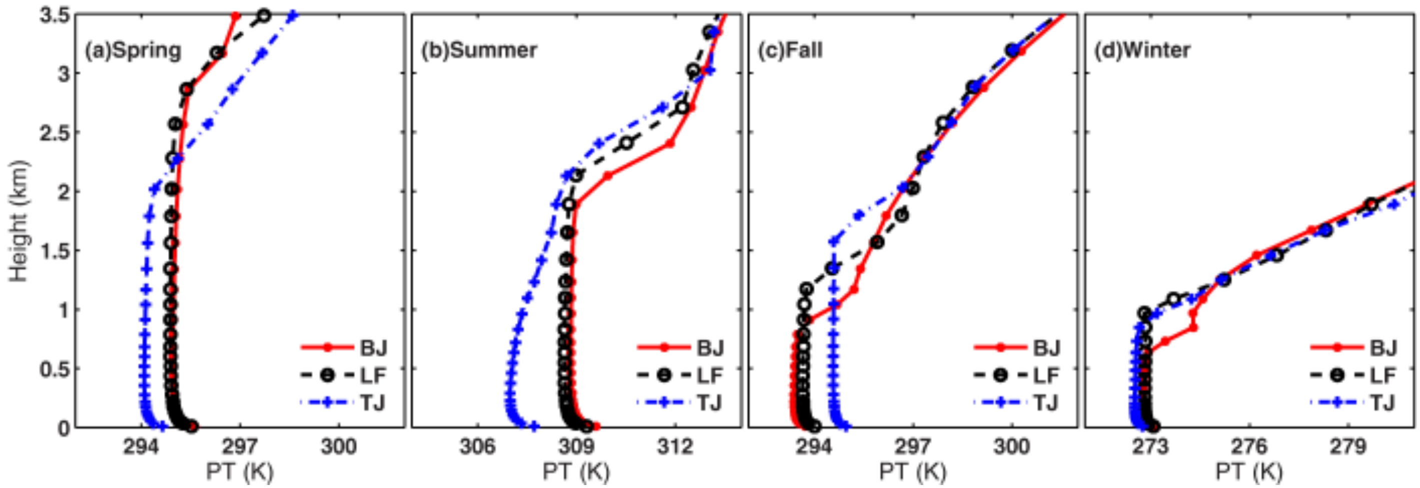
Impact of Mountain-Plain solenoid on boundary layer

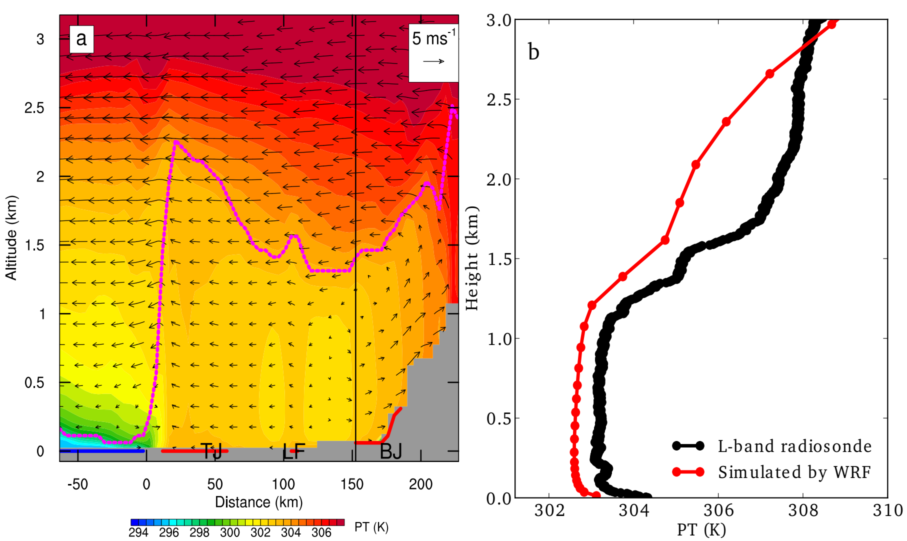


Mountain-Plain solenoid suppress boundary layer development and enhance air pollution (Hu et al., 2014, STE)

Impact of thermal effects on boundary layer

Seasonal study for the Beijing-Tianjin-Hebei region





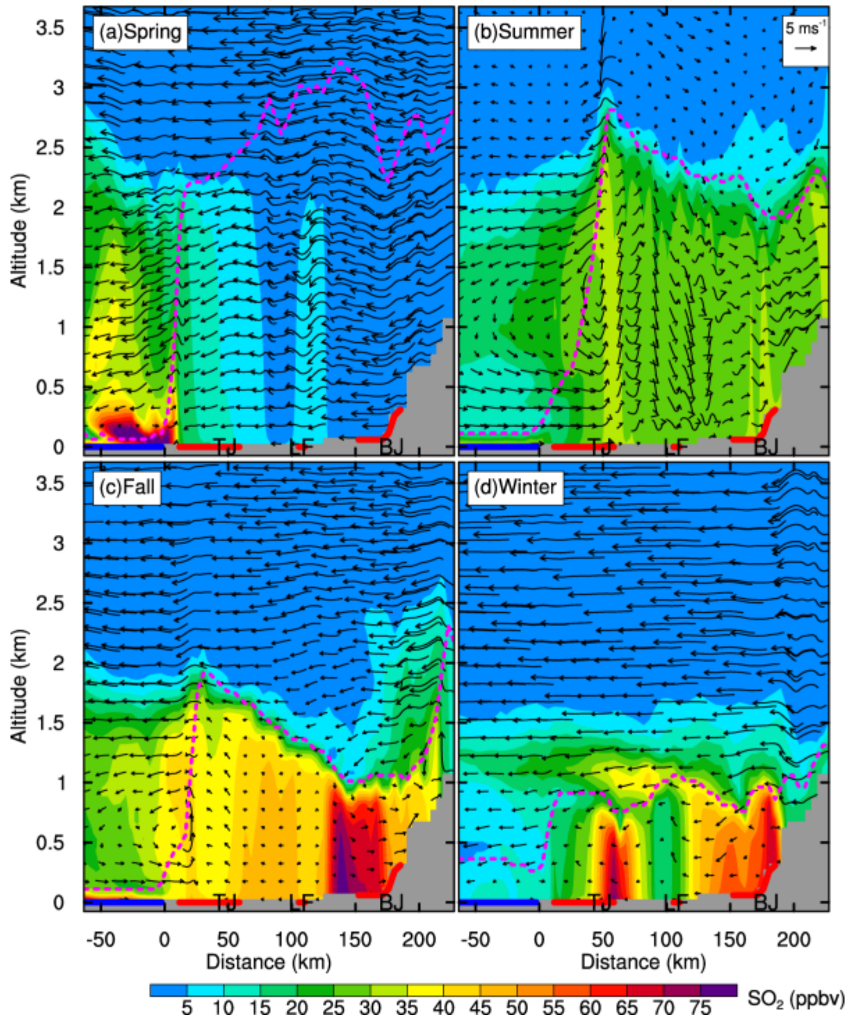
Thermal effects of Plateau partially lead to PBL height spring > summer > fall > winter

Miao and Hu et al. (2015, *JAMES*)

12 September 2010 simulated by WRF and observed by the L-band radiosonde.

Impact of thermal effects

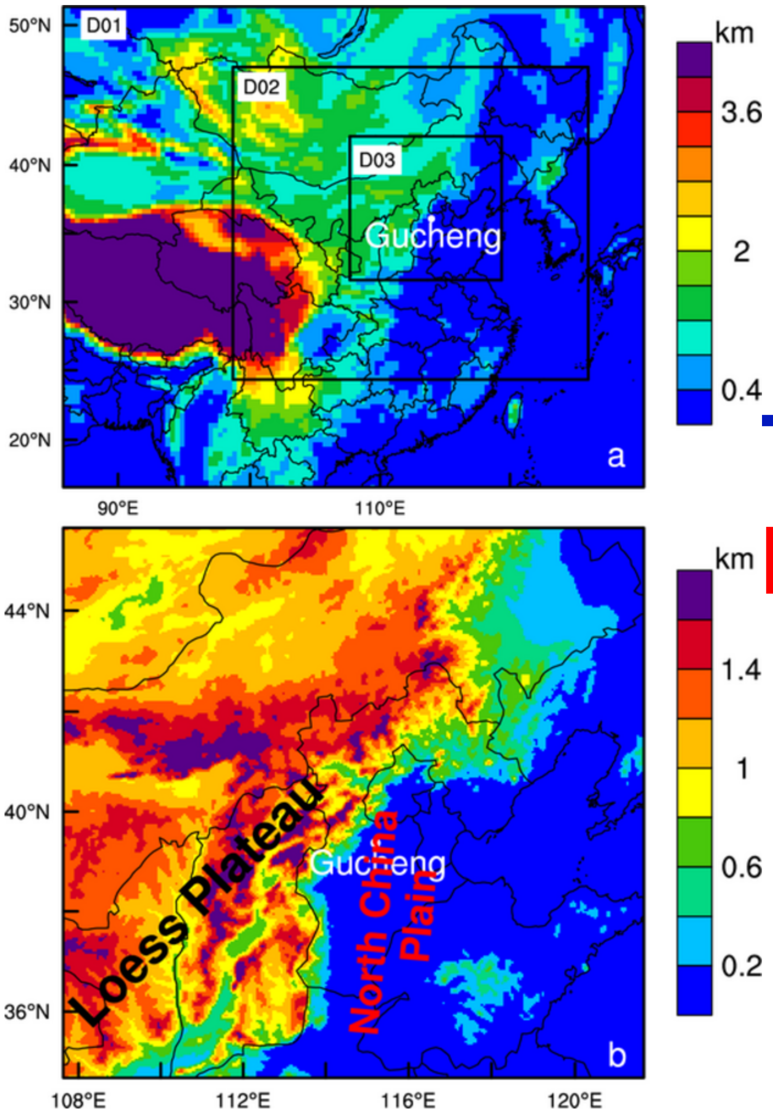
Seasonal variation of pollutants in the boundary layer



Thermal effects of Plateau partially lead to frequent haze events in Fall and Winter

Miao and Hu et al. (2015, *JAMES*)

Effects of Loess Plateau



Thermal (active*) effect

Dynamic (passive) effect

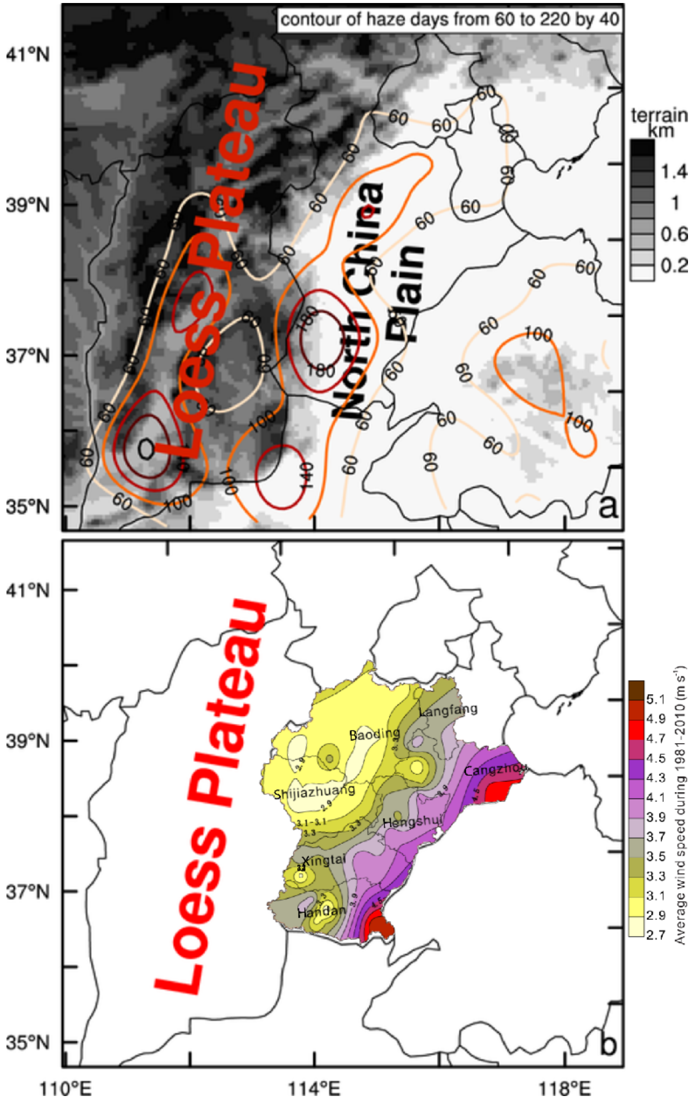
Dynamic effect of Loess Plateau

Hu, Li and Xue (2016a, BLM)*

- **Identify the dynamic effects of Loess Plateau**
- **Investigate the impact of such effects on air quality in the North China Plain (NCP)**

*Hu, X.-M., et al. (2016a), The Formation of Barrier Winds East of the Loess Plateau and their Effects on Dispersion Conditions in the North China Plains, *Bound.-layer meteor.*, DOI:10.1007/s10546-016-0159-4 .

Spatial distribution of haze days & wind speed



Weak winds in the west of NCP (Fu et al. 2014) **lead to** more frequent haze events in this region (Wu et al. 2014)

Fu GQ et al. (2014) The distribution and trends of fog and haze in the North China Plain over the past 30 years. Atmos Chem Phys 14:11949–11958.
Hu, X.-M., et al. (2016), The Formation of Barrier Winds East of the Loess Plateau and their Effects on Dispersion Conditions in the North China Plains, *Bound.-layer meteor.*, DOI:10.1007/s10546-016-0159-4 .
Wu D et al. (2014) The long-term trend of haze and fog days and the surface layer transport conditions under haze weather in North China. Acta Sci Circumst 34:1–11

Develop a slab model to simulate winds in NCP

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} + fv - g\frac{\partial h}{\partial x} - \phi_x\ , \qquad (1)$$

$$\frac{\partial v}{\partial t} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} - fu - g\frac{\partial h}{\partial y} - \phi_y\ , \qquad (2)$$

$$h = -\tau H\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right), \qquad (3)$$

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y}\ , \qquad (4)$$

C is the concentration of a passive pollutant
$H \approx 1$ km
h is the perturbation height of the layer top,
representing the pressure perturbation caused by mountain blocking and subsequent flow rising

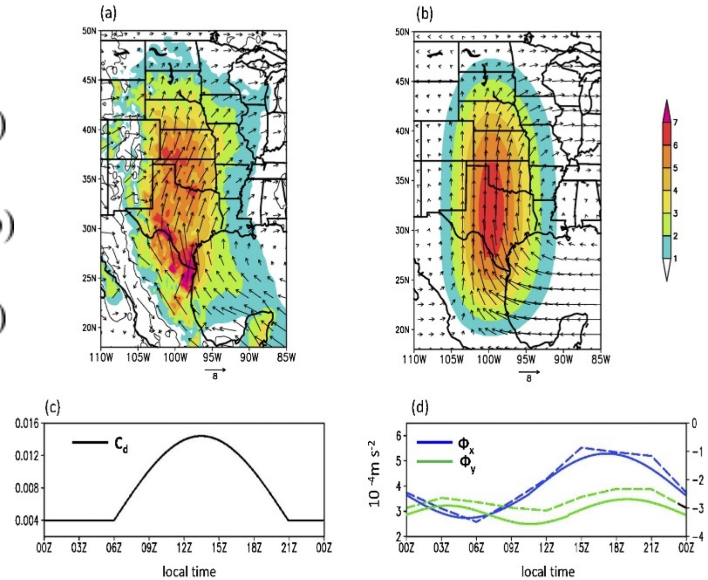
A slab model based on Pu and Dickinson (2014)

Pu and Dickinson (2014, JAS)

$$\frac{\partial u}{\partial t} = fv - g\frac{\partial h'}{\partial x} - \varepsilon u - \phi_x, \qquad (1a)$$

$$\frac{\partial v}{\partial t} = -fu - g\frac{\partial h'}{\partial y} - \varepsilon v - \phi_y, \qquad (1b)$$

$$h' = -\tau H\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right), \qquad (1c)$$



Hu (2016, BLM)

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} + fv - g\frac{\partial h}{\partial x} - \phi_x, \qquad (1)$$

$$\frac{\partial v}{\partial t} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} - fu - g\frac{\partial h}{\partial y} - \phi_y, \qquad (2)$$

$$h = -\tau H\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right), \qquad (3)$$

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y}, \qquad (4)$$

1. Removed friction
2. Added advection
3. Added pollutants

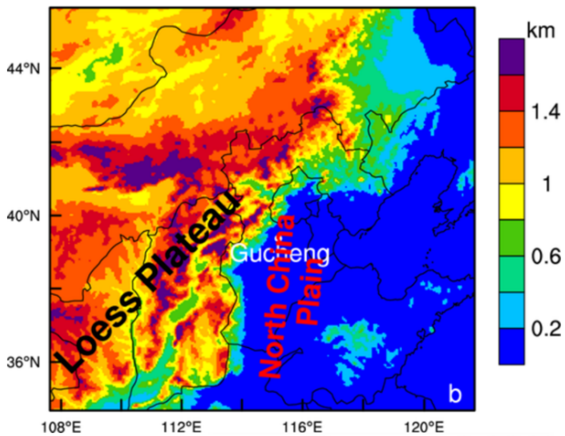
Model configuration of the slab model

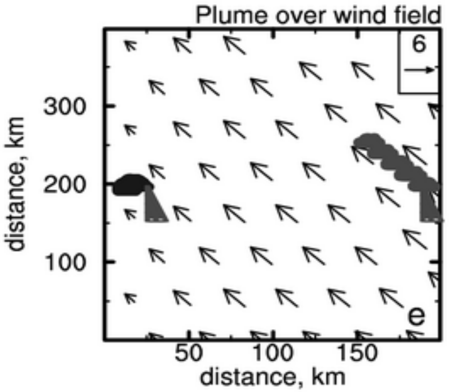
$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} + fv - g\frac{\partial h}{\partial x} - \phi_x , \quad (1)$$

$$\frac{\partial v}{\partial t} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} - fu - g\frac{\partial h}{\partial y} - \phi_y , \quad (2)$$

$$h = -\tau H\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right), \quad (3)$$

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} , \quad (4)$$





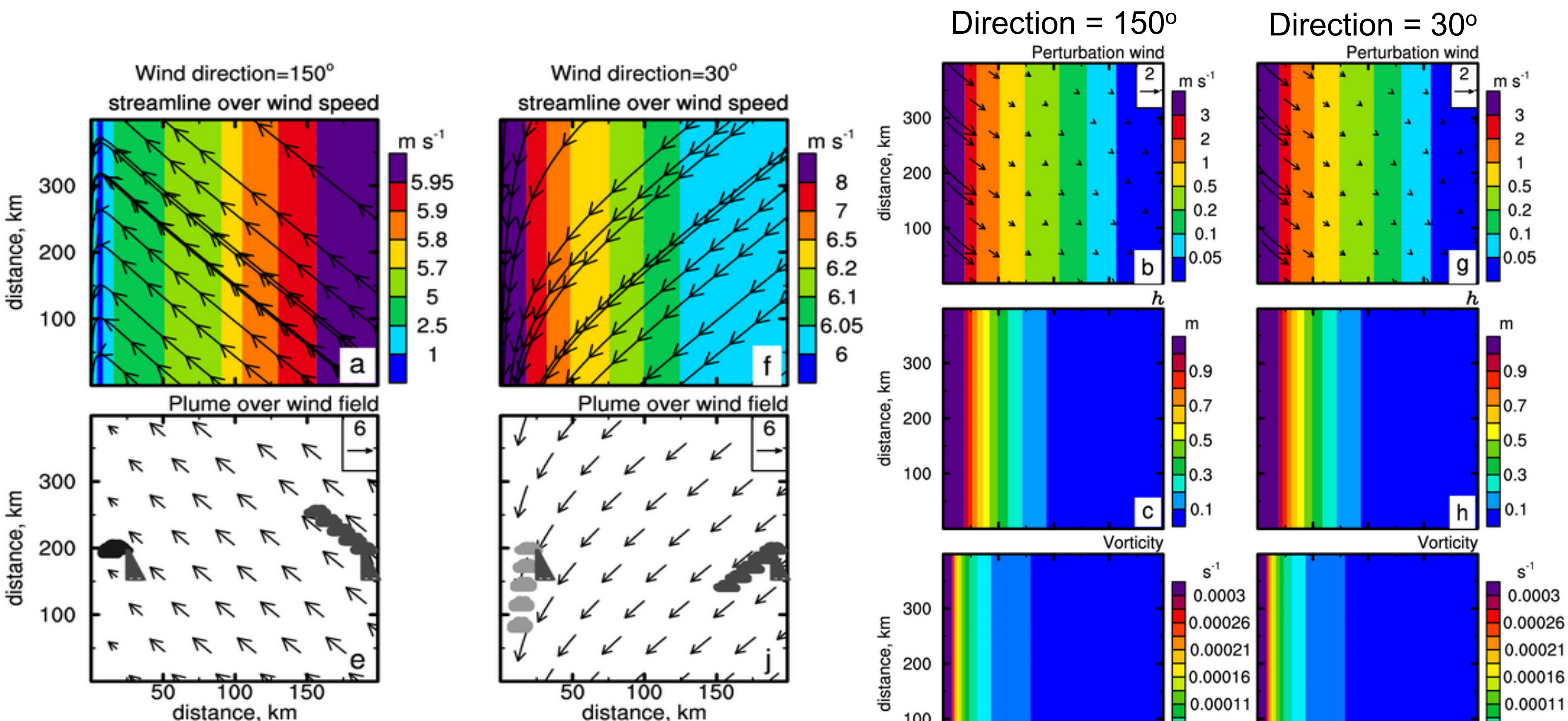
Domain: 400kmx400km

Boundary condition: slip-wall in west boundary
open condition in east

Ambient wind: 150^{o}C (southeasterly)
30^{o}C (northeasterly)

Geopotential gradient: constant

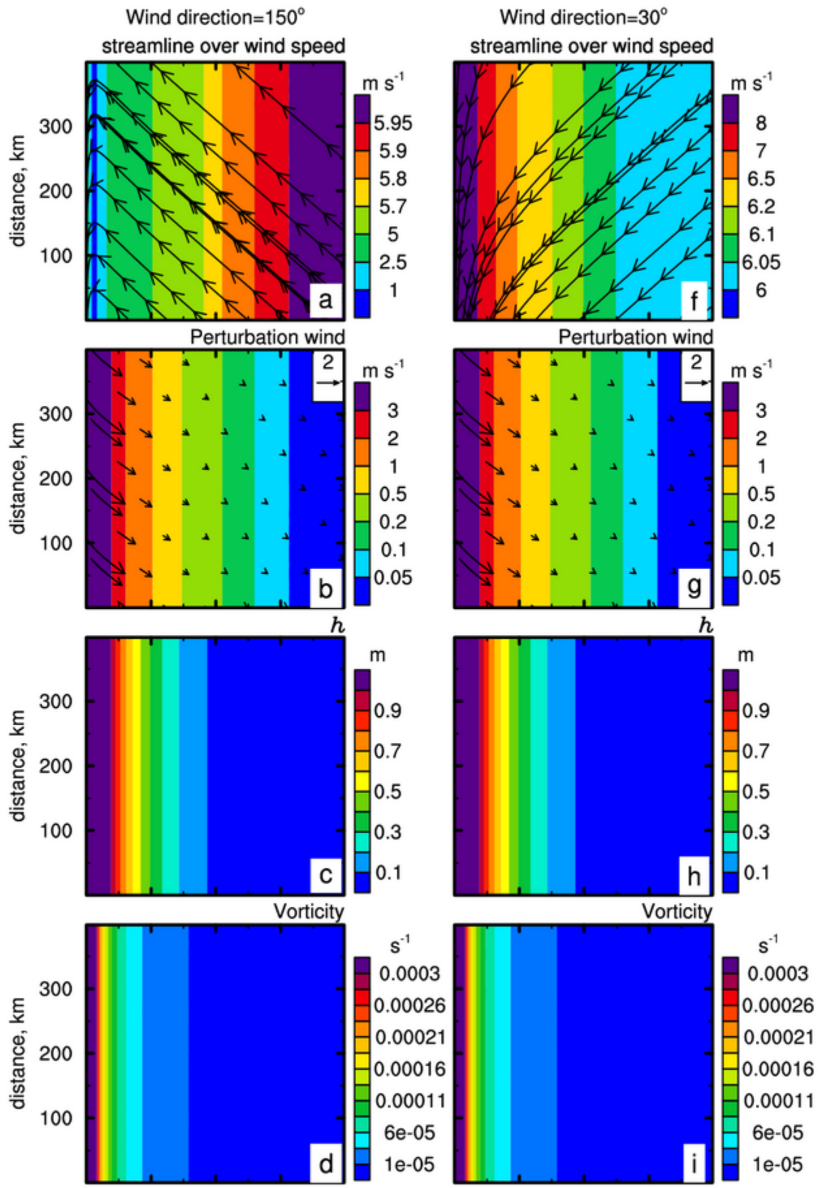
Simulated winds in NCP under 2 conditions



Same perturbation winds lead to different spatial distribution of wind speed.

- **Weak wind region for 150°C, leading to poor dispersion!**
- Barrier jet for 30°C, good dispersion!

Use vorticity budget to explain cyclonic turning of wind



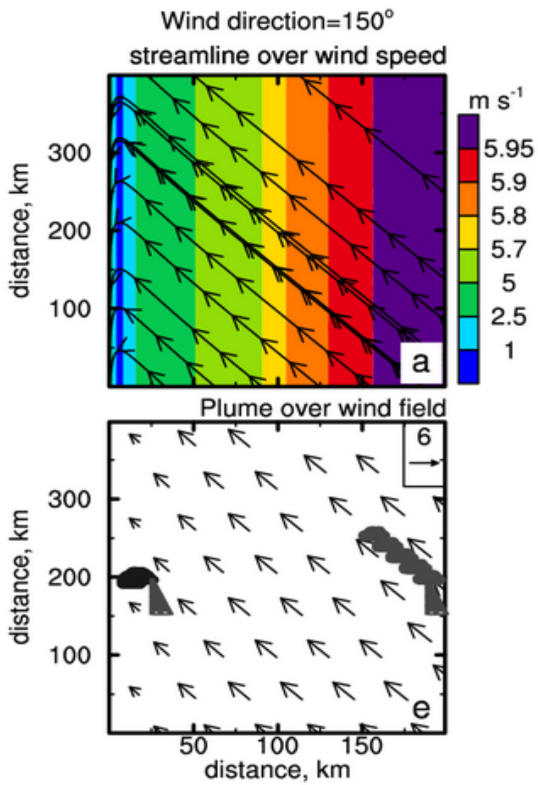
$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} + fv - g\frac{\partial h}{\partial x} - \phi_x \,, \quad (1)$$

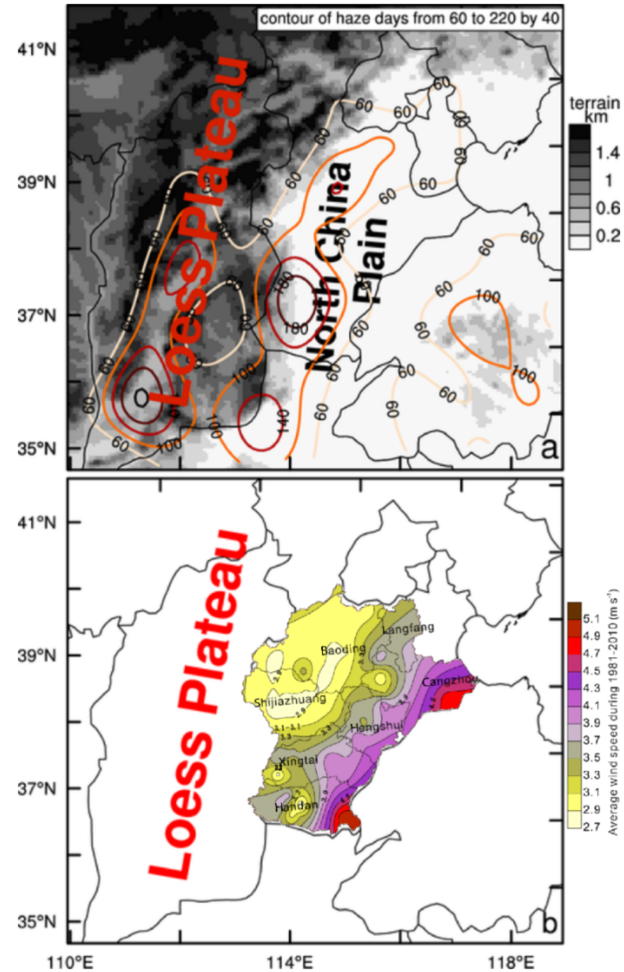
$$\frac{\partial v}{\partial t} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} - fu - g\frac{\partial h}{\partial y} - \phi_y \,, \quad (2)$$

Taking ∂/∂x of Eq. 2 and subtracting ∂/∂y of Eq. 1 gives the rate of relative vorticity

$$\frac{\partial \zeta}{\partial t} = -u\frac{\partial \zeta}{\partial x} - v\frac{\partial \zeta}{\partial y} - (\zeta + f)\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)$$

Impact on air quality in NCP





Weak wind region for southeasterly winds, leading to poor dispersion!

Conclusions for NCP

1.The Mountain-Plains Solenoid (MPS) circulation suppresses the mixed layer, exacerbating air pollution over the NCP

2.Thermal effects lead to seasonal variation of boundary layer and pollutants (more haze in fall and winter)

3.A one-layer slab model is developed to investigate the wind field in the North China Plain (NCP)

4. Dynamic modification by the Loess Plateau leads to barrier wind formation in the NCP

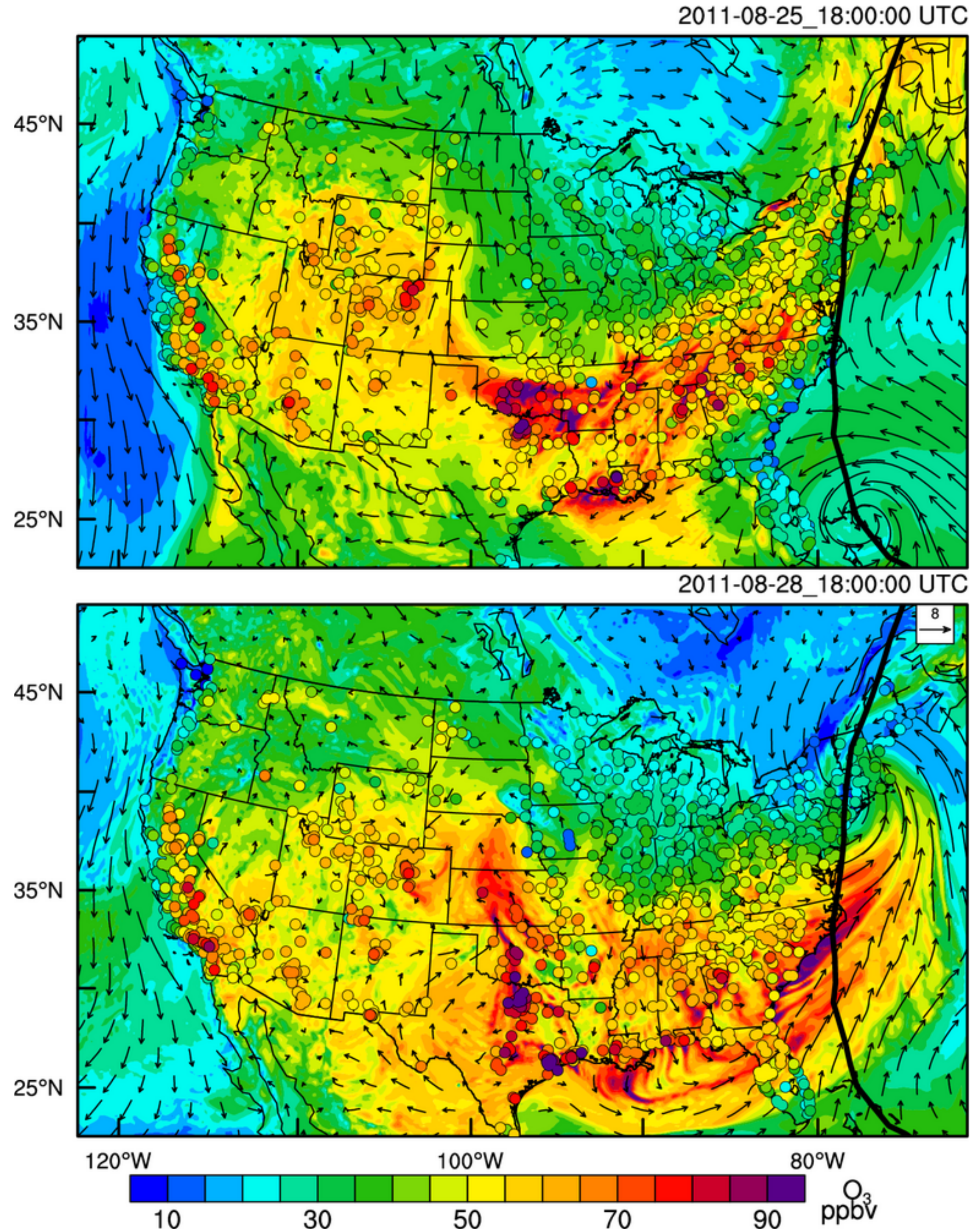
5. Barrier wind formation reduces the wind speed in the western part of NCP, leading to poor dispersion condition and exacerbating air pollution.

1. **0D gas phase mechanism model**
   to simulate O_3 over ocean
2. **1D chemistry model**
   to simulate impact of boundary layer processes
3. **Slab dispersion model**
   to investigate air quality in the NCP
4. **SREF-WRF/Chem ensemble system**
   to investigate air quality in Dallas

Aug 25-30, interesting O_3 episode

Area	Monitoring Site	POC	August 2011																														
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
Dallas-Fort Worth																																		
	Ft. Worth Northwest C13/AH302	2	54	65	64	55	50	45	45	36	45	41	41	39	31	69	56	47	53	52	54	61	60	54	50	56	82	81	86	87	73	66	58
	Keller C17	2	69	80	80	68	63	58	55	48	57	49	50	48	40	76	70	58	67	62	64	73	74	68	63	70	100	97	95	103	88	78	70
	Frisco C31/C680	1	86	80	92	78	65	61	54	52	62	47	42	45	43	68	77	57	68	67	71	79	65	73	70	71	91	92	78	89	83	76	72
	Midlothian OFW C52/A137	1	50	63	61	56	50	42	41	40	42	37	43	36	29	74	58	46	49	57	58	66	57	47	54	60	65	72	95	81	80	71	60
	Denton Airport South C56/A163/X157	1	73	86	86	77	66	62	59	52	54	53	45	48	44	70	74	61	70	60	67	72	74	76	63	66	102	87	81	98	90	76	71
	Arlington Municipal Airport C61	1	55	66	67	58	50	44	44	39	44	38	43	37	26	74	61	45	49	54	56	63	53	51	53	57	69	73	92	83	77	68	59
	Dallas North No.2 C63/C679	1	81	78	87	69	58	53	48	46	50	41	41	38	44	68	68	50	59	64	64	75	67	64	64	67	90	98	88	86	82	73	67
	Rockwall Heath C69	1	80	76	91	69	56	48	46	42	47	42	44	40	57	61	67	36	45	54	54	67	59	49	52	56	65	79	73	65	64	66	56
	Grapevine Fairway C70/A301/X182	1	71	83	86	73	60	NV	NA	NV	56	44	45	42	37	68	71	53	64	61	64	71	69	68	62	67	98	91	87	97	81	72	64
	Kaufman C71/A304/X071	1	58	65	65	57	60	54	44	36	40	42	41	41	47	60	60	54	50	56	60	66	65	50	58	52	62	76	81	68	73	74	64
	Granbury C73/C681	1	45	59	60	55	48	41	41	37	43	39	49	35	37	67	51	44	49	51	52	59	53	48	50	53	61	70	82	80	71	67	56
	Eagle Mountain Lake C75	1	55	70	67	59	53	49	48	37	45	47	39	38	36	74	59	49	59	52	55	62	65	59	52	56	84	75	79	85	73	63	58
	Parker County C76	1	52	67	69	63	56	50	50	41	49	47	58	39	45	70	62	55	61	58	59	67	68	59	56	61	84	78	88	93	82	72	63
	Cleburne Airport C77/C682	1	50	60	60	56	50	43	41	38	43	41	44	38	37	74	50	43	48	54	56	62	52	50	52	57	67	69	90	82	75	67	56
	Dallas Hinton St. C401/C60/AH161	3	70	75	75	61	52	48	44	41	43	35	41	33	34	68	59	45	40	52	55	67	60	55	55	58	79	88	90	84	76	66	58
	Dallas Executive Airport C402	1	60	70	69	55	48	41	40	37	42	34	41	32	30	69	58	44	47	55	59	67	58	51	56	57	71	78	96	82	82	73	63
	Greenville C1006/A198	1	70	67	80	64	52	49	46	38	44	36	41	45	38	69	74	50	54	61	65	71	64	54	58	59	73	83	77	73	66	76	66
	Pilot Point C1032	1	78	88	91	84	75	68	60	60	64	56	42	51	50	71	91	65	75	67	74	79	64	79	72	67	91	87	79	92	81	83	77
	Italy C1044/A323	1	43	54	56	52	44	38	33	37	36	35	43	33	34	58	57	47	46	55	57	66	57	49	53	59	62	NV	83	75	79	71	60
	Corsicana Airport C1051	1	54	64	61	56	58	51	40	37	39	42	43	38	27	64	61	53	57	59	61	67	58	57	59	57	63	69	84	70	76	78	66

A severe O3 pollution event in DFW during the passage of Hurricane Irene, 2011

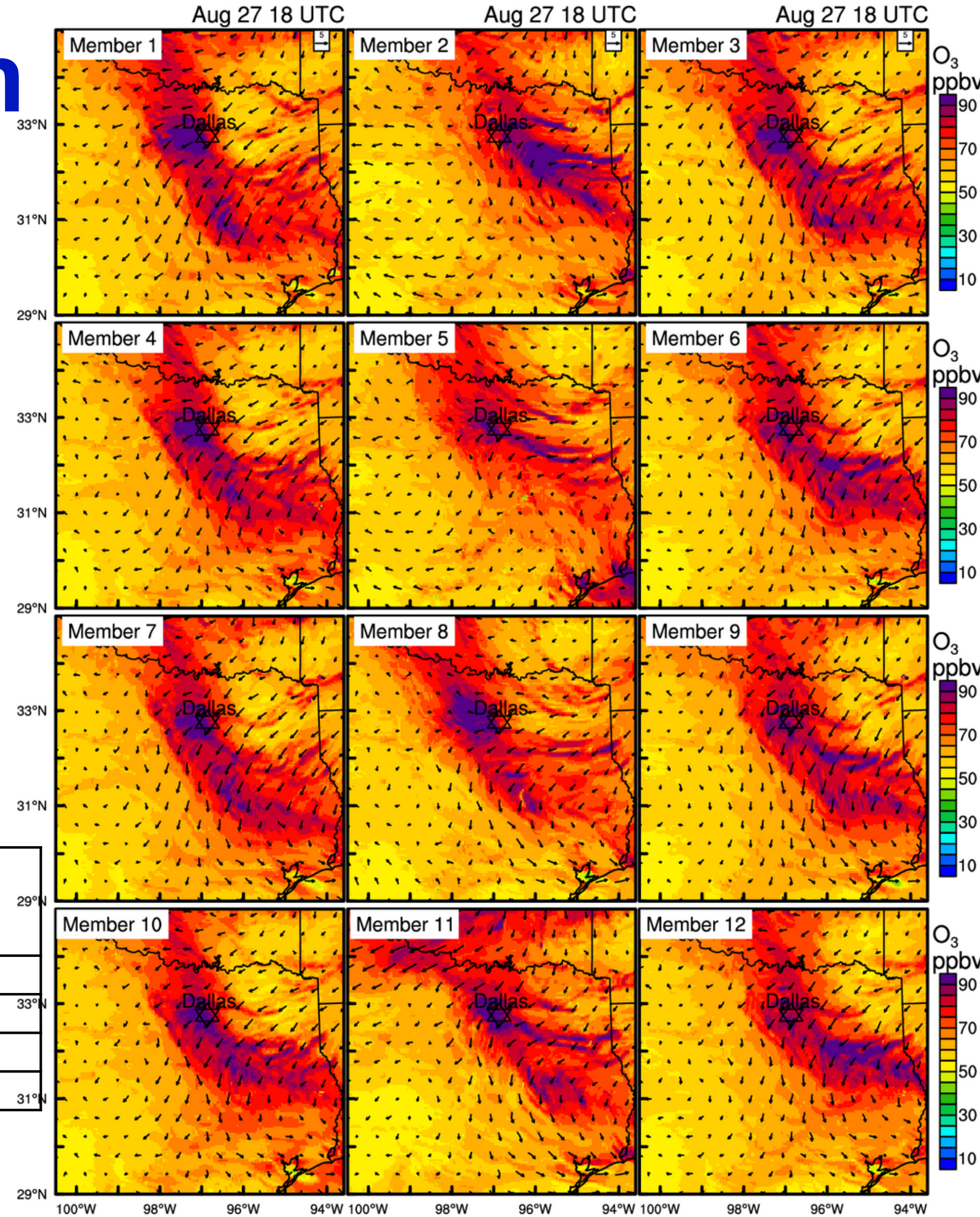


SREF-WRF/Chem Ensemble O_3 prediction

The 12 ensemble members differ by their driving meteorological fields

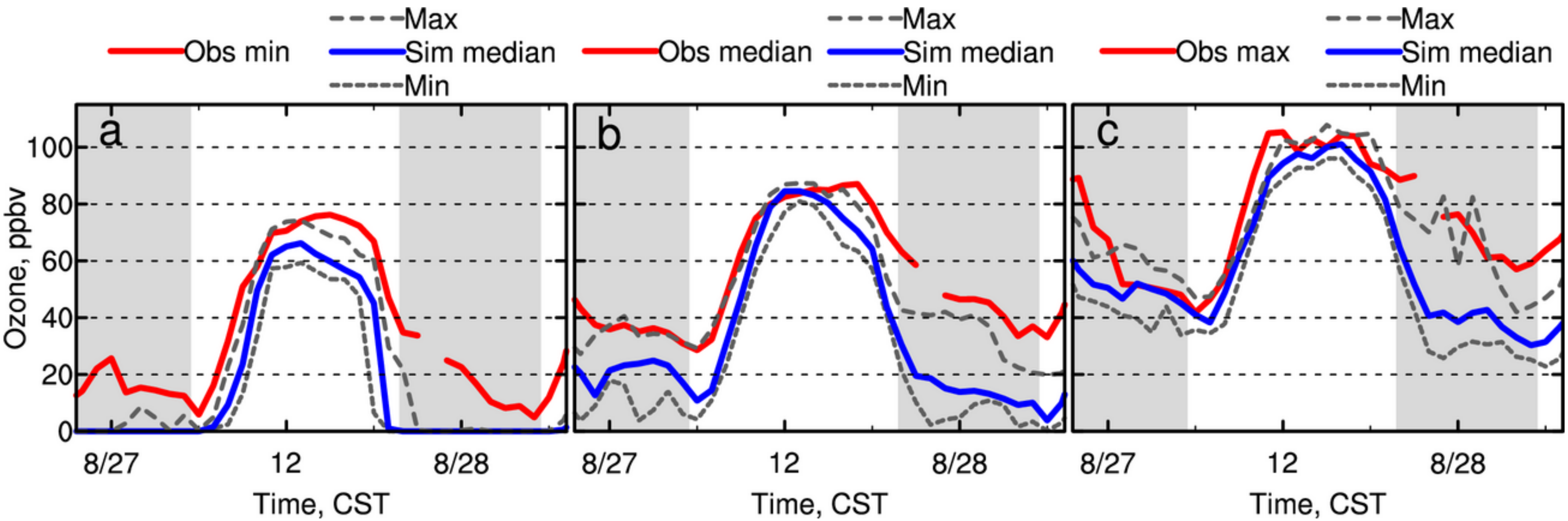
Table 1. Details of the 12 SREF members used in the SREF-WRF/Chem ensemble system*

Models / Perturbations	EM	Eta	NMM
n1	Member 1	Member 2	Member 3
n2	Member 4	Member 5	Member 6
P1	Member 7	Member 8	Member 9
p2	Member 10	Member 11	Member 12



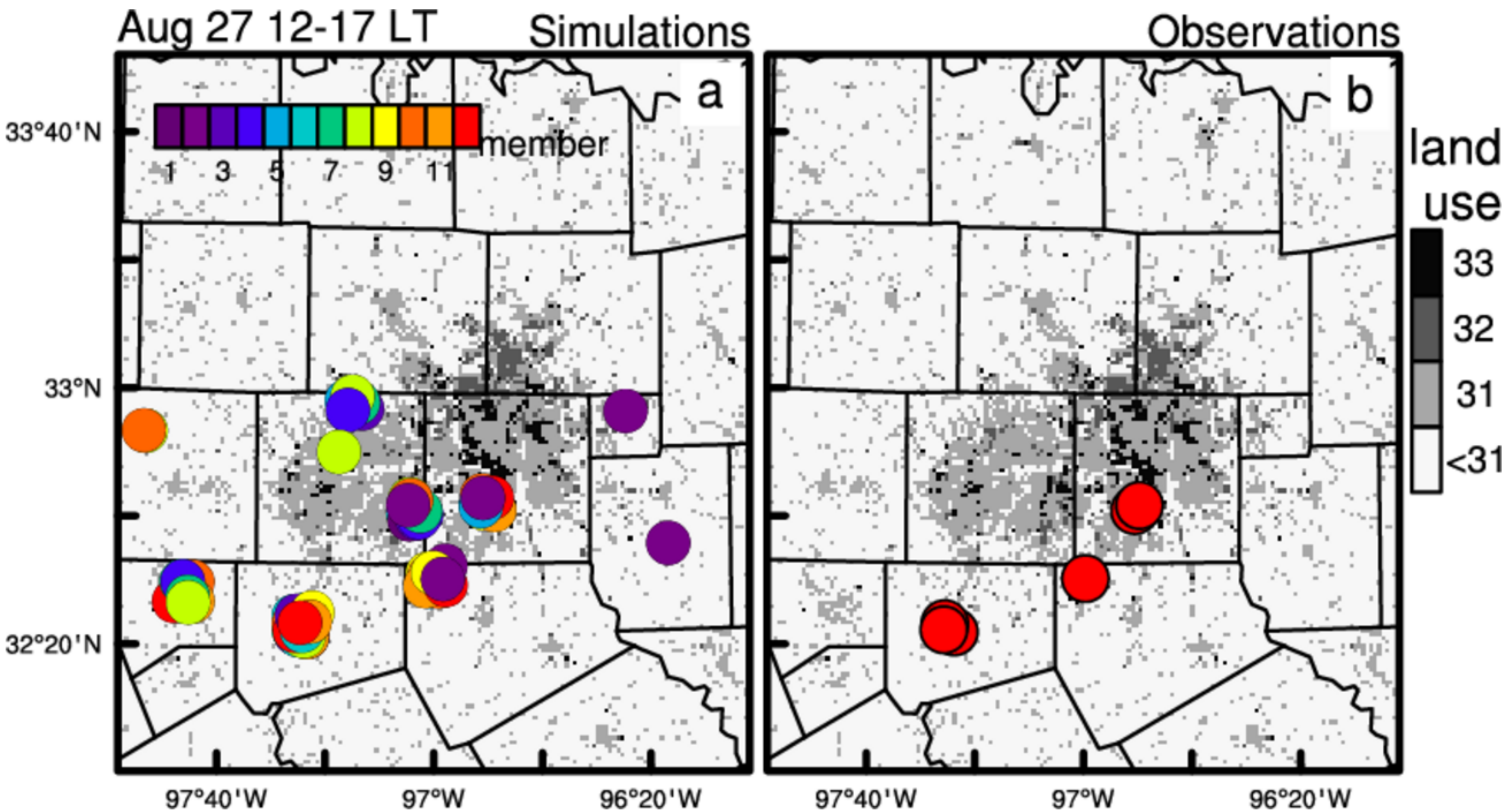
Short-Range Ensemble Forecast (SREF)

Capability to capture min, median, max O_3 in DFW?



Underestimation of nighttime O_3 due to deficiency of the coupling between the meteorological and chemical components in WRF/Chem

Simulated and observed locations with maximum O_3



Ensemble mean did better in terms of plume direction

Conclusions

1. The stagnant zone associated with Hurricane passage confined the pollutant plume emanated from DFW, leading to prominent boundary layer O_3 formation.

2. Ensemble SREF-WRF/Chem prediction are conducted to examine the impact of transport uncertainties on air quality forecasting. The ensemble mean gives a better prediction in terms of plume directions.

References

1. **Hu, X.-M.**, X. Li, M. Xue, D. Wu et al. (2016a), The Formation of Barrier Winds East of the Loess Plateau and their Effects on Dispersion Conditions in the North China Plains, Bound.-layer meteor., DOI:10.1007/s10546-016-0159-4
2. **Hu, X.-M.**, and M. Xue (2016b), Influence of synoptic sea breeze fronts on the urban heat island intensity in Dallas-Fort Worth, Texas, *Mon. Wea. Rev.*, doi:10.1175/MWR-D-15-0201.1.
3. **Hu, X.-M.**, M. Xue, et al. (2016c), Analysis of Urban Effects in Oklahoma City using a Dense Surface Observing Network, *J. Appl. Meteor. Climatol.*, doi:10.1175/JAMC-D-15-0206.1 .
4. **Hu, X.-M.**, et al. (2014), Impact of the Loess Plateau on the Atmospheric Boundary Layer Structure and Air Quality in the North China Plain: A Case Study, Science of the Total Environment, 10.1016/j.scitotenv.2014.08.053
5. Miao, Y., **X.-M. Hu**, et al. (2015), Seasonal variation of local atmospheric circulations and boundary layer structure in the Beijing-Tianjin-Hebei region and implications for air quality, *J. Adv. Model. Earth Syst.*, DOI: 10.1002/2015MS000522.
6. **Hu, X.-M.**, et al. (2013), Impact of Low-Level Jets on the Nocturnal Urban Heat Island Intensity in Oklahoma City. *J. Appl. Meteor. Climatol.*, 52, 1779–1802.
7. **Hu, X.-M.**, et al. (2013), Enhanced vertical mixing associated with a nocturnal cold front passage and its impact on near-surface temperature and ozone concentration, *J. Geophys. Res.*, 118, 2714– 2728.
8. **Hu, X.-M.**, P. Klein , M. Xue, F. Zhang, D. Doughty, R. Forkel, E. Joseph, and J. D. Fuentes (2013), Impact of the Vertical Mixing Induced by Low-level Jets on Boundary Layer Ozone Concentration, *Atmos. Environ.*, 70, 123-130
9. **Hu, X.-M.**, J. M. Sigler, and J. D. Fuentes (2010), Variability of ozone in the marine boundary layer of the equatorial Pacific Ocean , *J. of Atmos. Chem.*, 66, 117–136.