

# The sensitivity of ozone and its precursors to PBL transport parameterizations within the WRF-Chem model

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## *Acknowledgements*

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Song-You Hong (Yonsei University)*



# Outline

1. Introduction of two PBL schemes in WRF-Chem model
2. YSU vs. MYJ in summer 2004 simulations
3. Model vs. NOAA-P3 aircraft obs. during ICARTT
4. Model vs. Ron Brown ship obs. during ICARTT and sensitivity of model to K parameterizations in YSU
5. Summary



**ICARTT: International Consortium for Atmospheric Research on Transport and Transformation**  
Field exp. during the summer of 2004 by groups in North America and Europe

# WRF-Chem model setup

- **Simulation period : Jun/1/2004~Aug/31/2004, daily 24 hour retrospective run**
- **Meteorological initial & boundary condition : NCEP GFS analysis field**
- **Domain : Eastern US**
- **Resolution : 27km (horizontal) / 16m~1.5km (vertical)**
- **PBL models : YSU & MYJ**
- **Land-surface model : Noah**
- **Microphysics : WSM5**
- **Cumulus parameterization : Grell-Devenyi**
- **Photolysis scheme : Madronich (1987)**
- **Chemistry : RADM2**

# PBL parameterizations in WRF-Chem model 1

YSU PBL : Troen and Mahrt (1986), Hong and Pan (1996), Noh et al. (2003)

$$\frac{\partial C}{\partial t} = \frac{\partial(-\overline{wc})}{\partial z} = \frac{\partial}{\partial z} \left[ K_c \left( \frac{\partial C}{\partial z} - \gamma_c \right) - \overline{wc}_h \left( \frac{z}{h} \right)^3 \right] \quad \text{for } z < h$$

↗ Entrainment flux

$C; U, V, \Theta, Q$       **Counter-gradient term (nonlocal mixing)**

$$K_h = \text{Pr}^{-1} k w_s z (1 - z/h)^2, \quad w_s = (u_*^3 + 7k w_*^3 z/h)^{1/3}$$

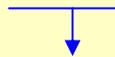
$0.01 \leq K_h \leq 1000 \text{ (m}^2 \text{ s}^{-1}\text{)}$       **Mixed-layer height info. is needed.**

$$Ri_b(z) = \frac{g(\Theta_v(z) - \Theta_s)z}{\Theta_{va} U(z)^2}, \quad \text{Critical } Ri_b = 0$$

**Under stable regime, pbl height ~ 1<sup>st</sup> model level  
→ K for free atmosphere is used!**

## PBL parameterizations in WRF-Chem model 2

**Mellor-Yamada-Janjic PBL** : Mellor and Yamada (1974, 1982), Janjic (1990)

$$\frac{D}{Dt} \left( \frac{q^2}{2} \right) + \dots = P_s + P_b - \varepsilon, \quad q^2 = u^2 + v^2 + w^2$$


**Turbulent Kinetic Energy**

$$l = l_0 kz(kz + l_0)^{-1}, \quad l_0 = \alpha \frac{\int_0^\infty |z| q dz}{\int_0^\infty q dz}, \quad \alpha = const$$

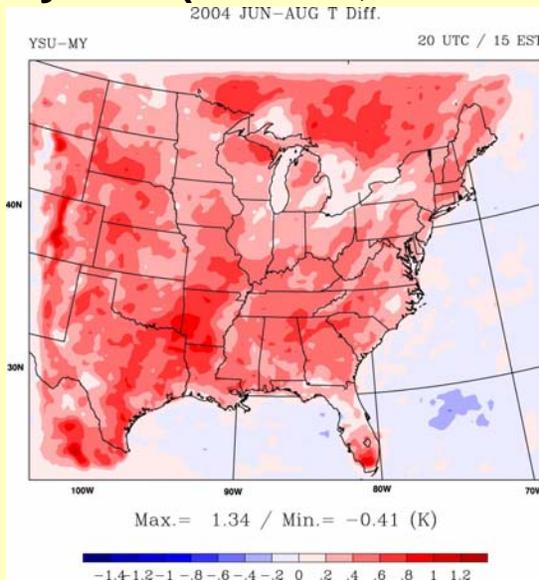
**Master length scale**

$$K_m = lqS_m, \quad K_h = lqS_h, \quad local\ mixing$$

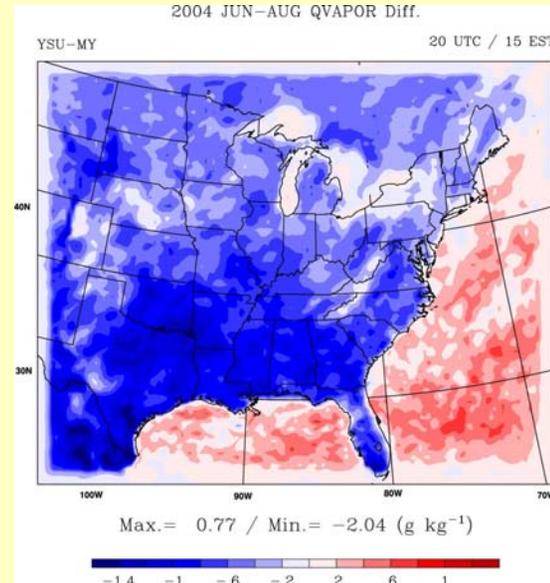
# YSU - MY During Summer 2004 : Meteorology

## Daytime (20 UTC, 15 EST)

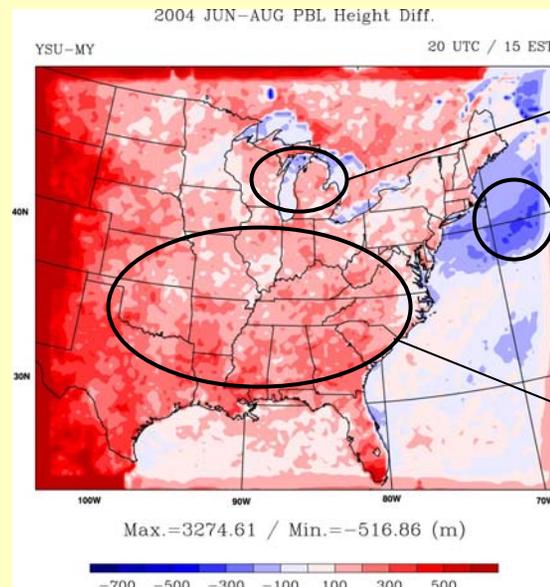
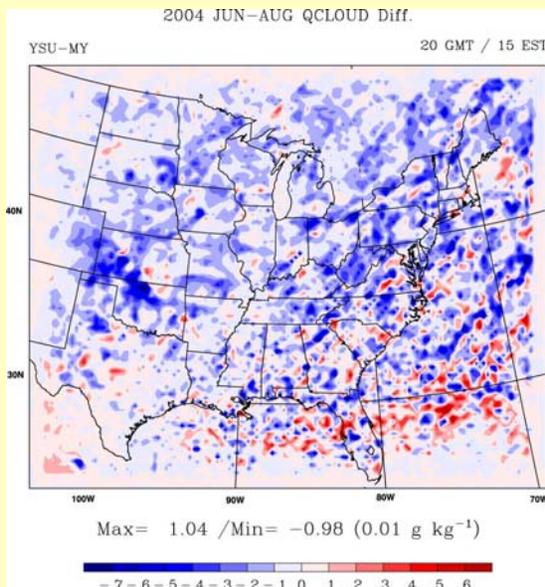
T



$q_v$



$q_c$



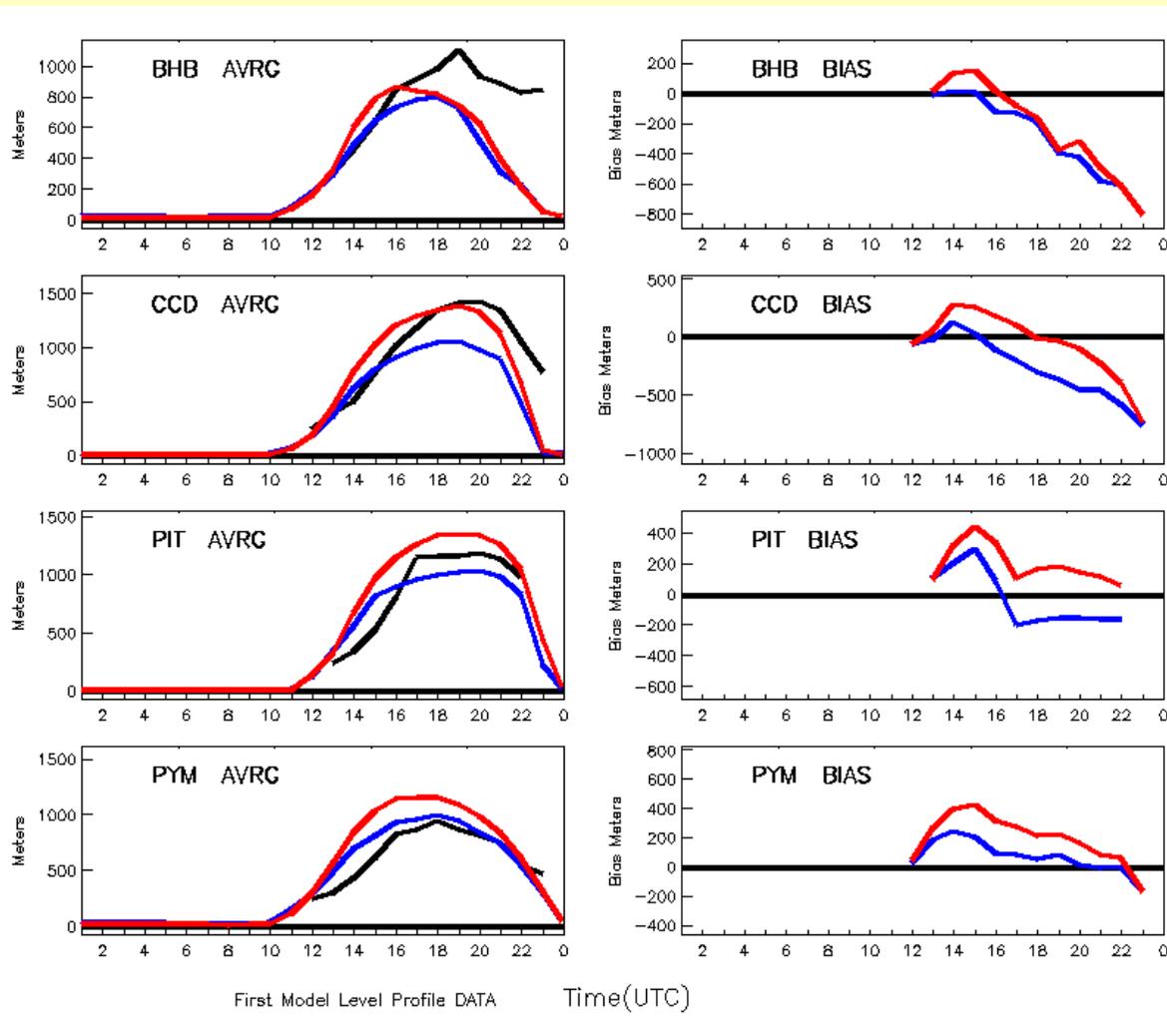
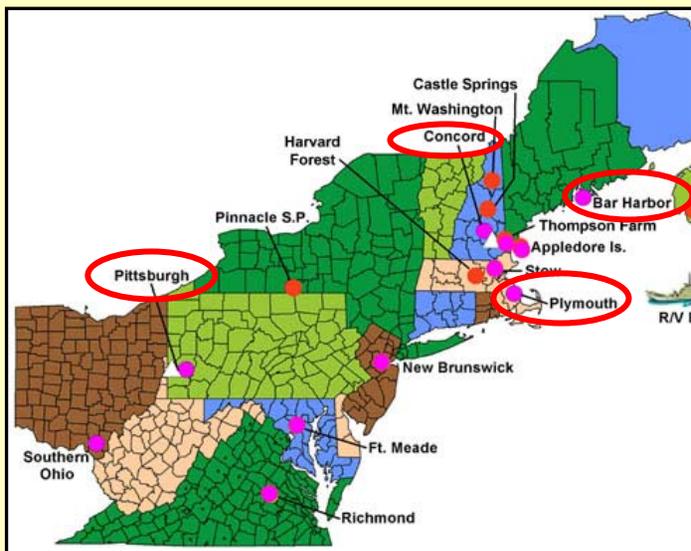
**YSU  
50-100%  
lower**

PBL  
Height

**YSU 10-30%  
higher**

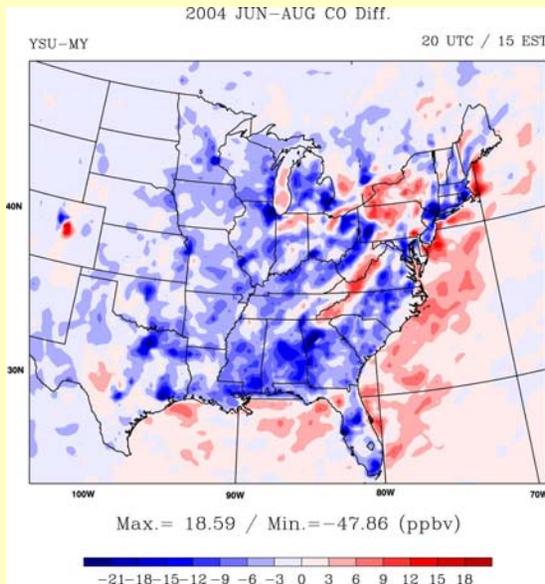
# CBL Height Evaluation with Wind Profiler Data

41 Days for 4 separate sites

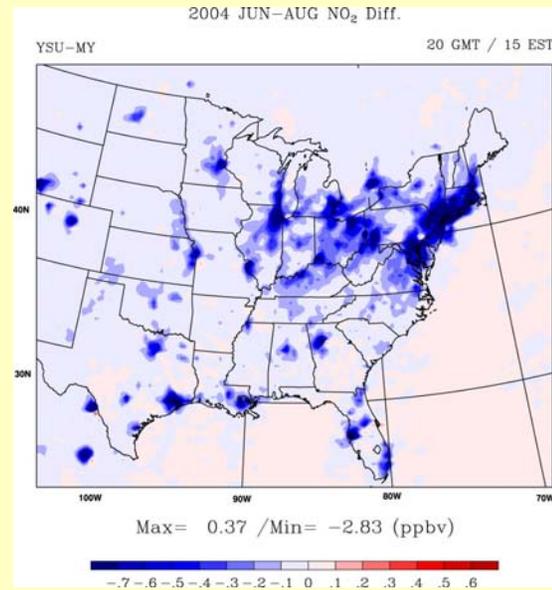


# YSU - MY During Summer 2004 : Chemical Species

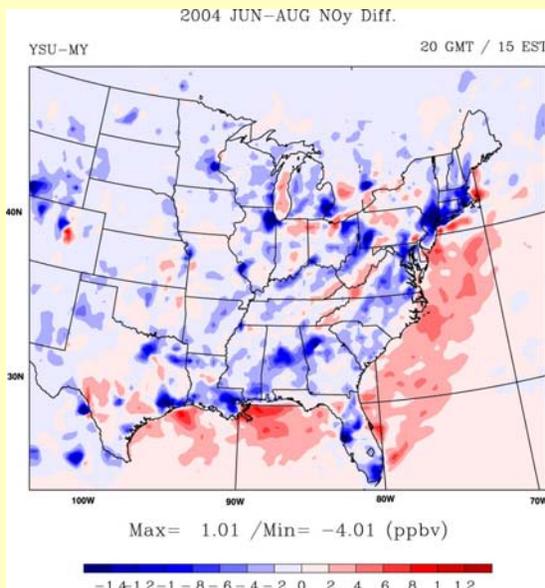
CO



NO<sub>2</sub>

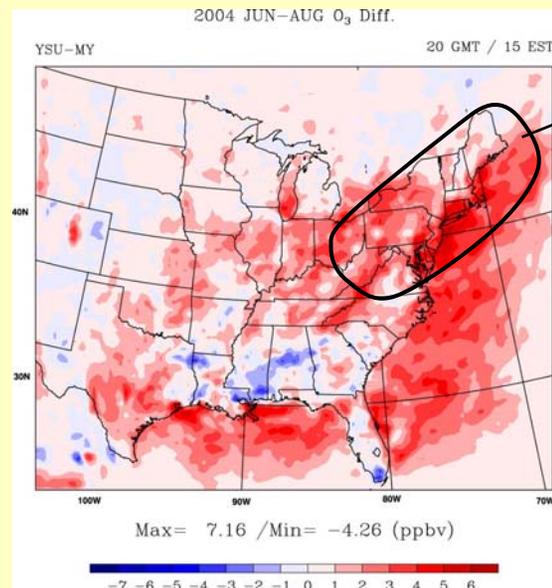


NO<sub>y</sub>



ICARTT  
domain

O<sub>3</sub>

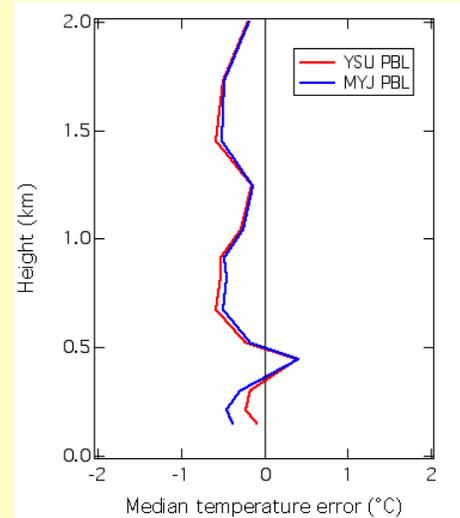
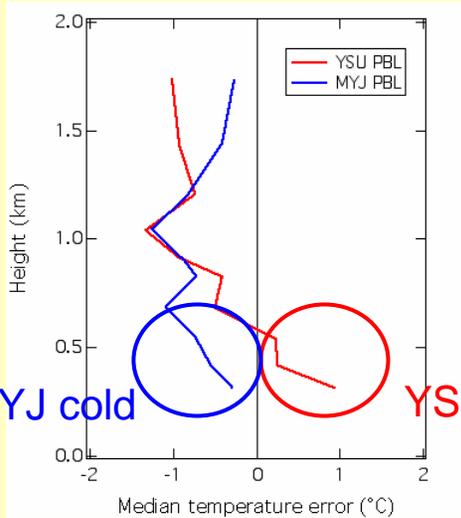


# Comparison with P3 Aircraft During ICARTT : T and $q_v$

## Daytime over land

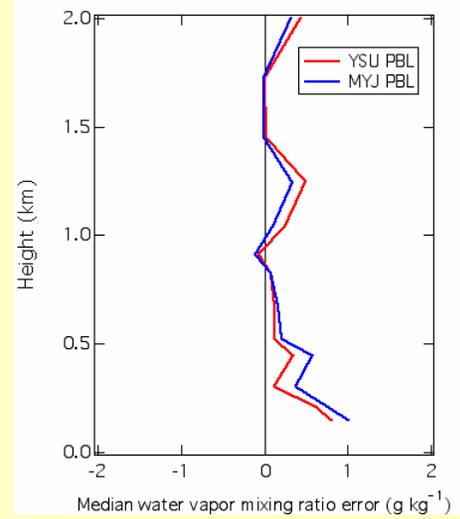
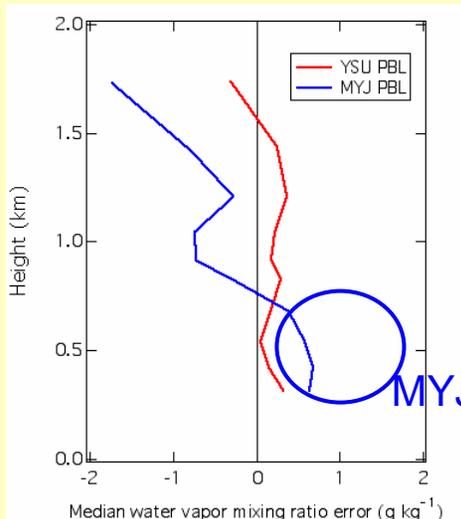
## Nighttime

T



T

$q_v$



$q_v$

### Note

\* 15 flights  
(7/15/04-  
8/15/04)

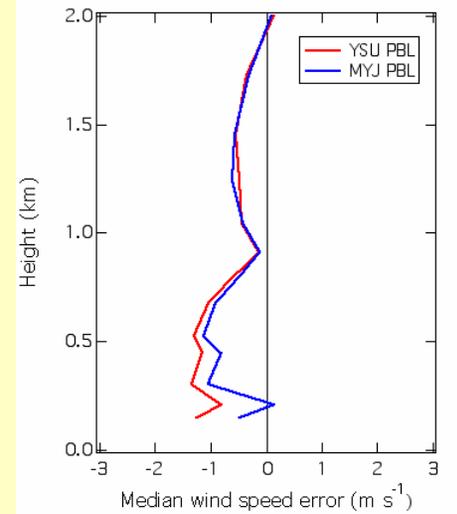
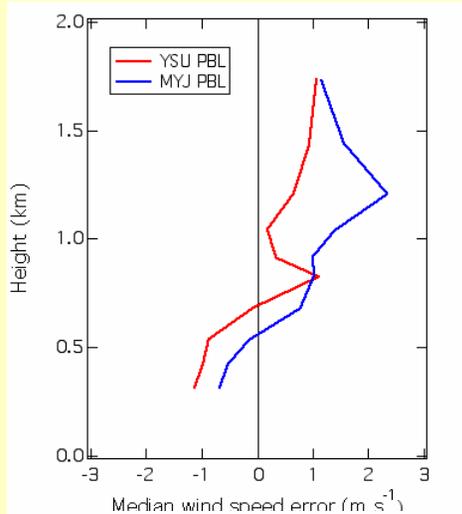
\* Median  
error

# Comparison with P3 Aircraft During ICARTT : **wind**

## Daytime over land

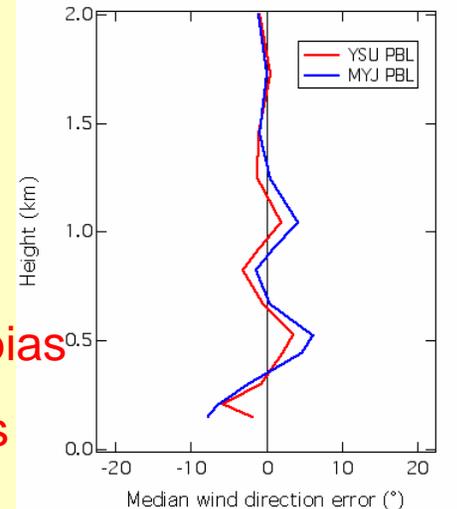
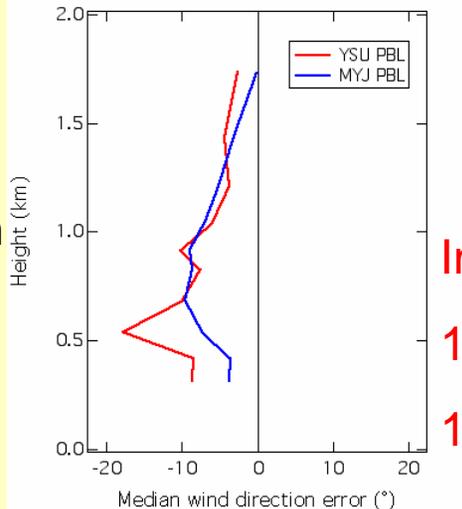
## Nighttime

Wind speed



Wind speed

Wind direction



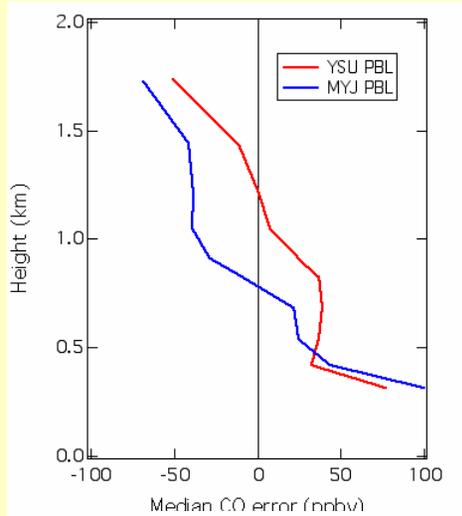
Wind direction

In lower BL,  
**1  $\text{ms}^{-1}$  low bias**  
**10 deg. bias**

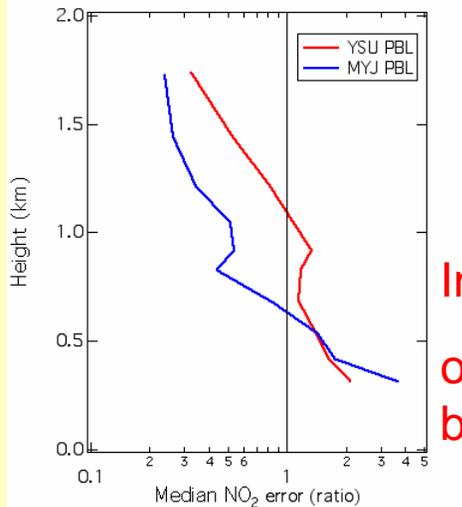
# Comparison with P3 Aircraft During ICARTT : CO & NO<sub>2</sub>

Daytime over land

CO



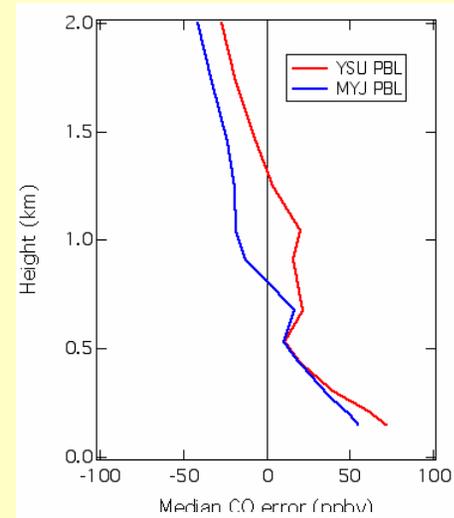
NO<sub>2</sub>



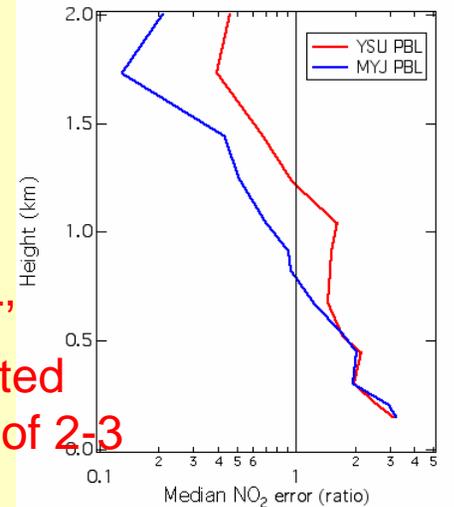
In lower BL,  
overestimated  
by a factor of 2-3

Nighttime

CO



NO<sub>2</sub>



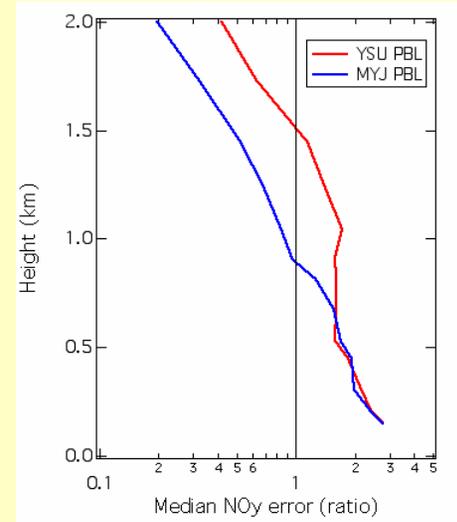
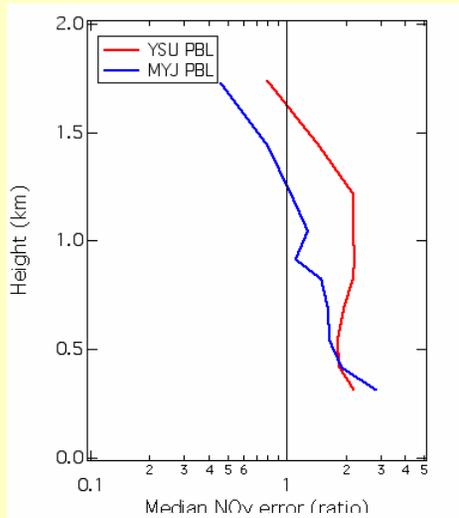
# Comparison with P3 Aircraft During ICARTT : $\text{NO}_y$ and isoprene

Daytime over land

Nighttime

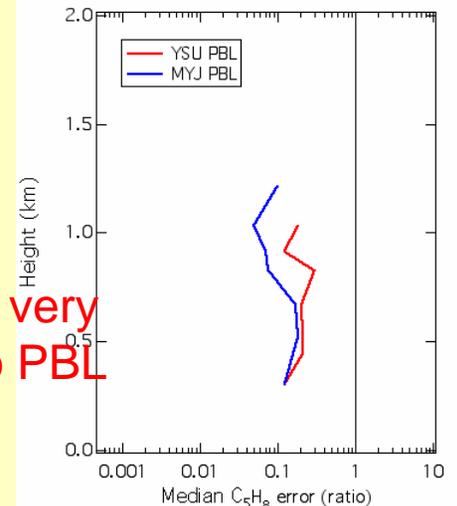
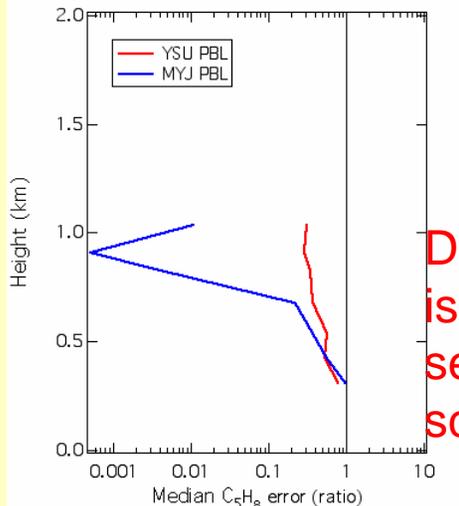
$\text{NO}_y$

$\text{NO}_y$



Isoprene

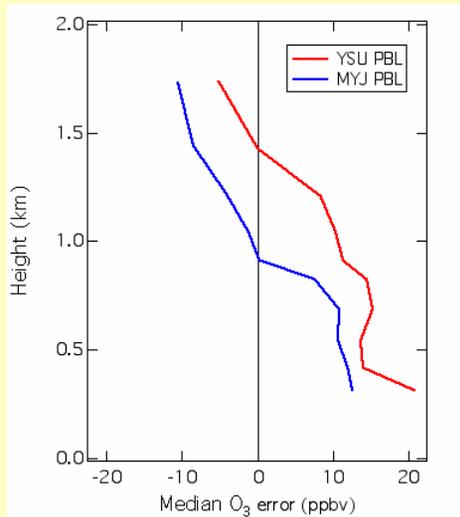
Isoprene



Daytime,  
isoprene is very  
sensitive to PBL  
scheme.

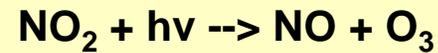
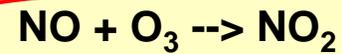
# Comparison with P3 Aircraft During ICARTT : $O_3$

Daytime  
over land

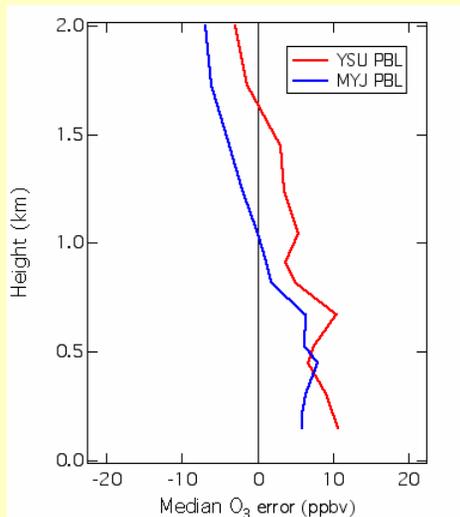


Increased  $NO_x$  results in lower  $O_3$ .

$NO_x$  titration



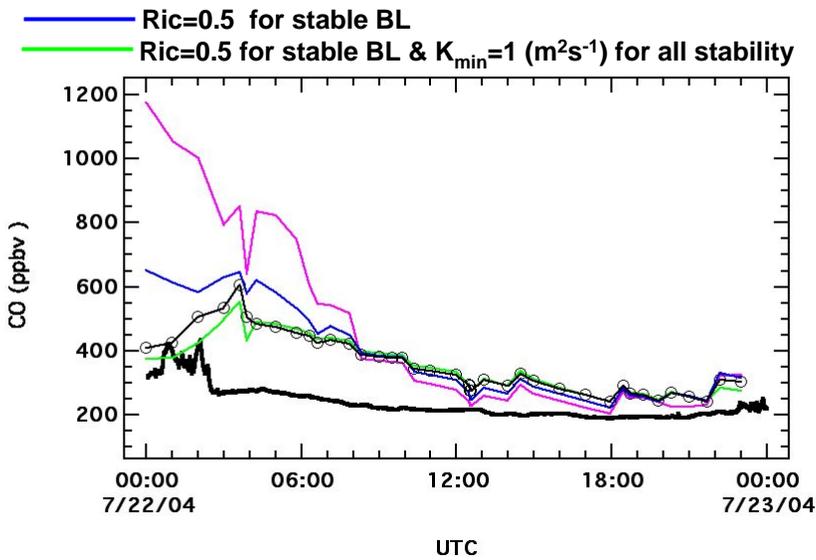
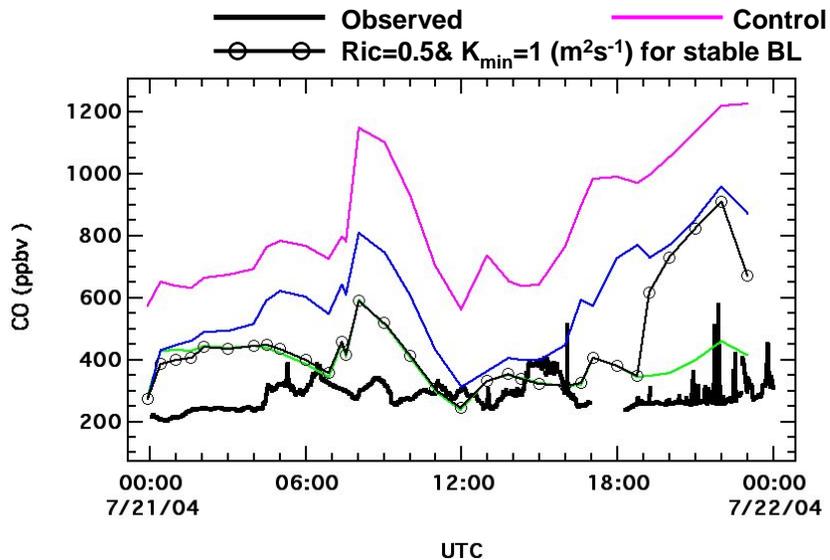
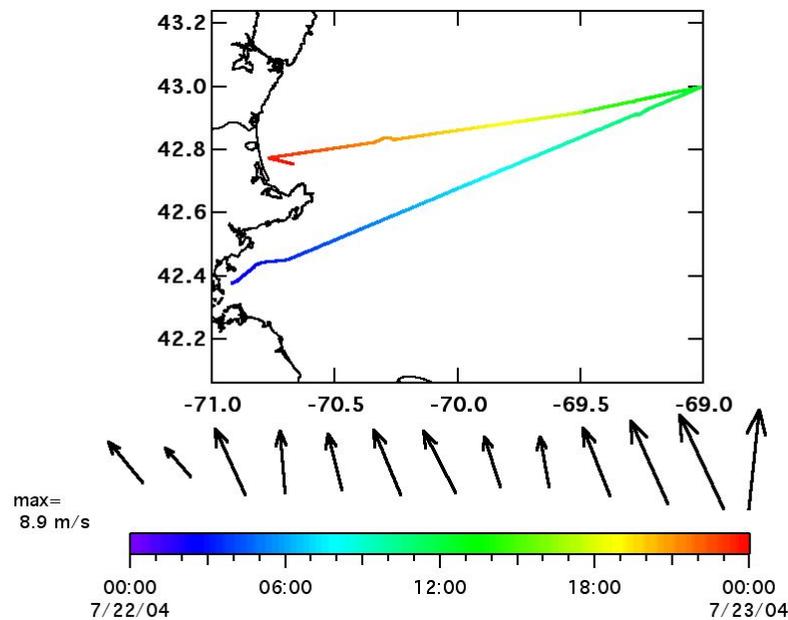
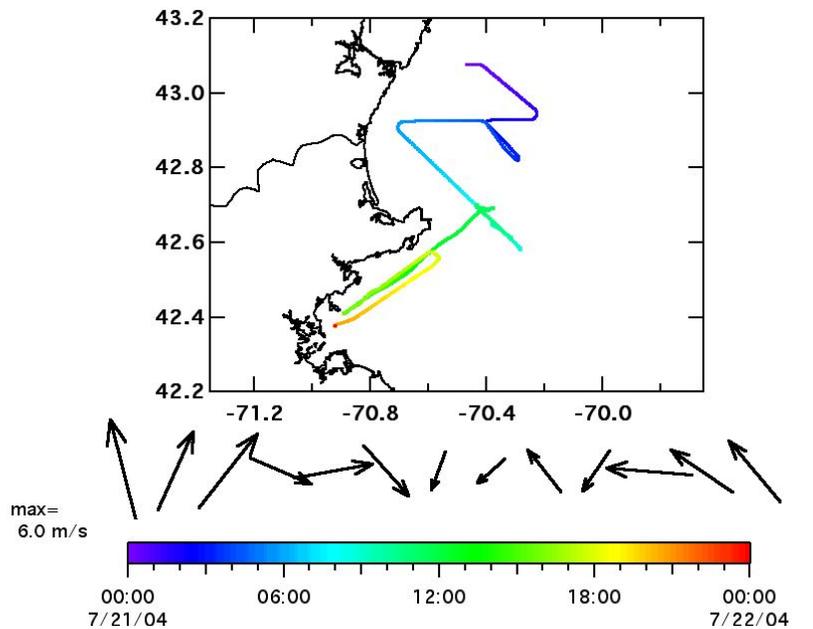
Nighttime



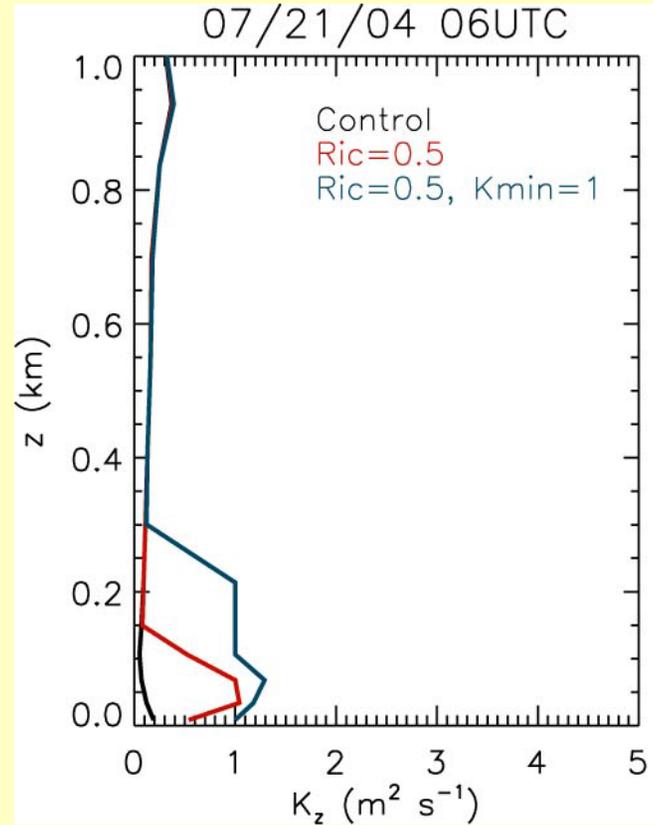
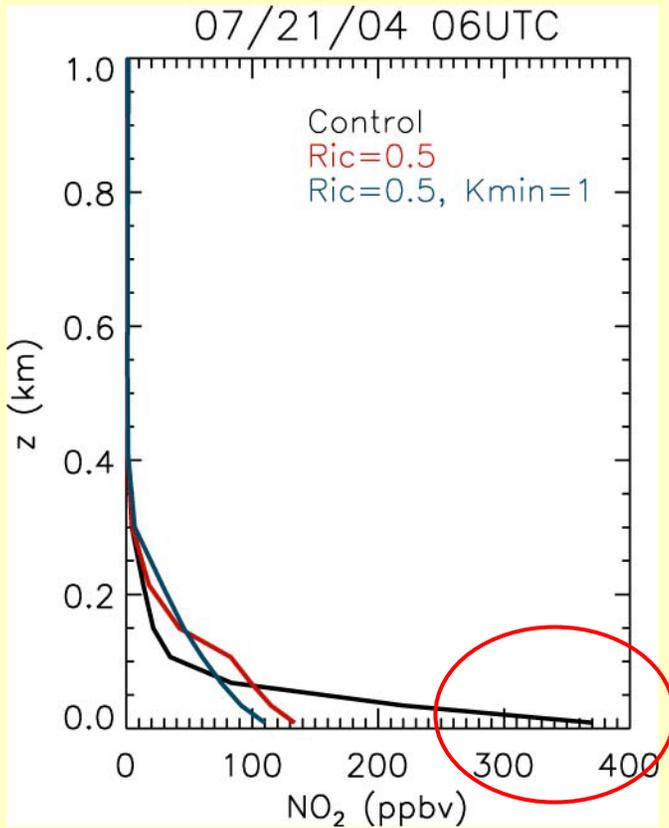
# Comparison with RB Ship Obs. During ICARTT : CO

Jul/21/04

Jul/22/04



# Vertical profile of model NO<sub>2</sub> and K over water : YSU



Sharp gradient  
near the surface

Max ~ 400 ppbv

# Summary

- 1. Aircraft & Ship measurements indicate poor chemical species mixing in the lower boundary layer**
- 2. Over land during daytime, CO, NO<sub>2</sub>, NO<sub>y</sub> in MYJ > those in YSU (except O<sub>3</sub>)**
- 3. Under stable regime (over water), chemical species mixing in both schemes is too much underestimated.**
- 4. Stable boundary layer representation in YSU PBL is being modified.**

# Future direction

1. Non-local mixing in chemical species

2. Fair-weather cumulus venting

3. Sensitivity to the vertical resolution



Daytime  
mixing

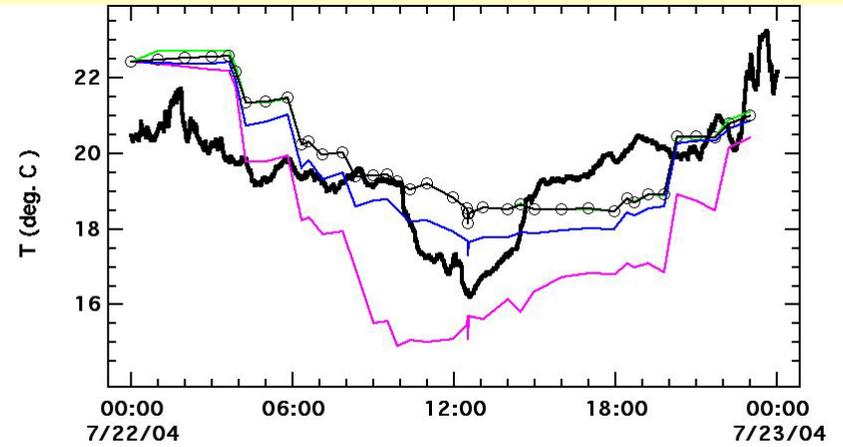
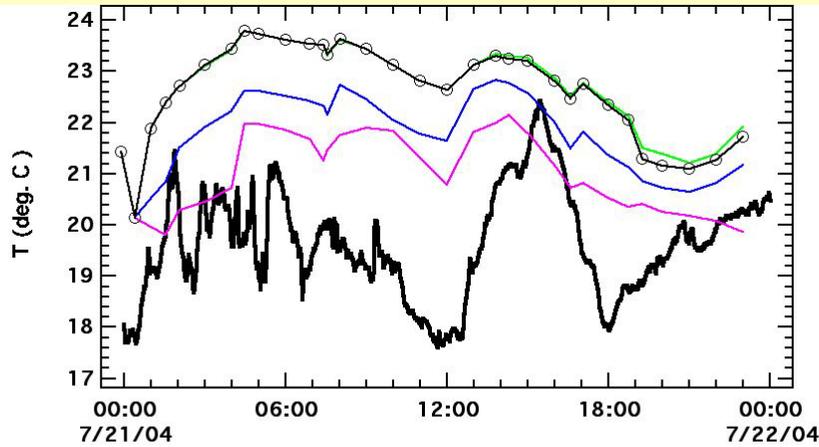


Emission, Stable BL

# Comparison with RB Ship Obs. During ICARTT : T & Q<sub>v</sub>

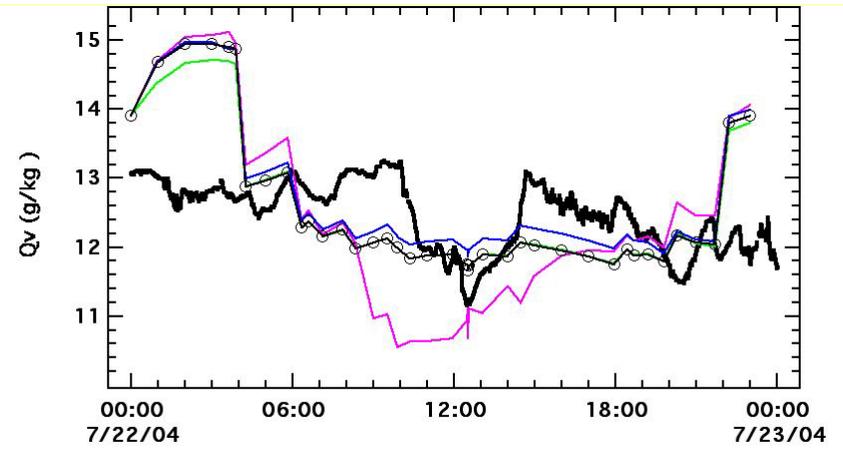
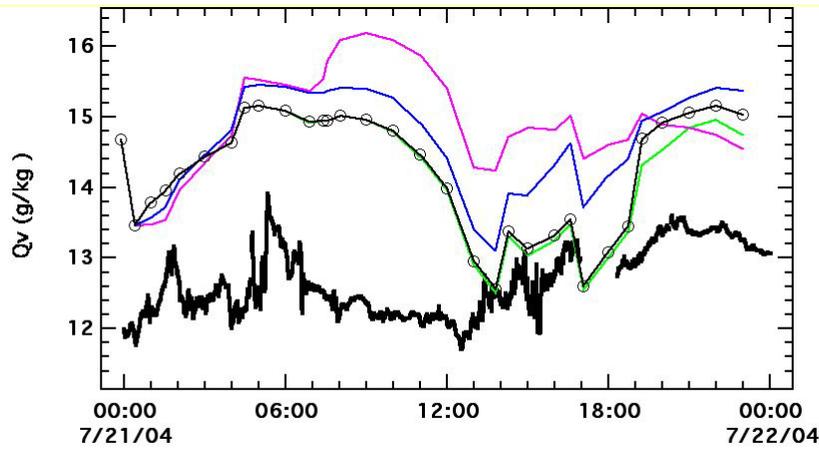
Jul/21/04

Jul/22/04



— Observed      — Control  
○—○ Ric=0.5 & K<sub>min</sub>=1 (m<sup>2</sup>s<sup>-1</sup>) for stable BL

— Ric=0.5 for stable BL  
— Ric=0.5 for stable BL & K<sub>min</sub>=1 (m<sup>2</sup>s<sup>-1</sup>) for all stability

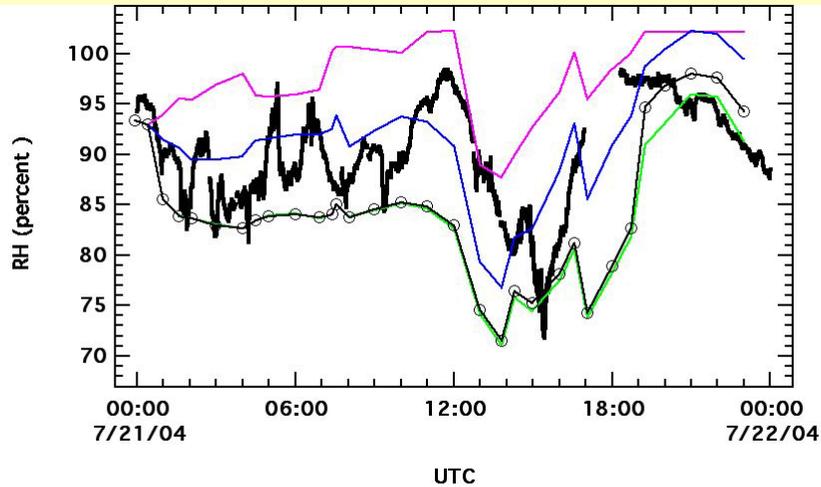


UTC

UTC

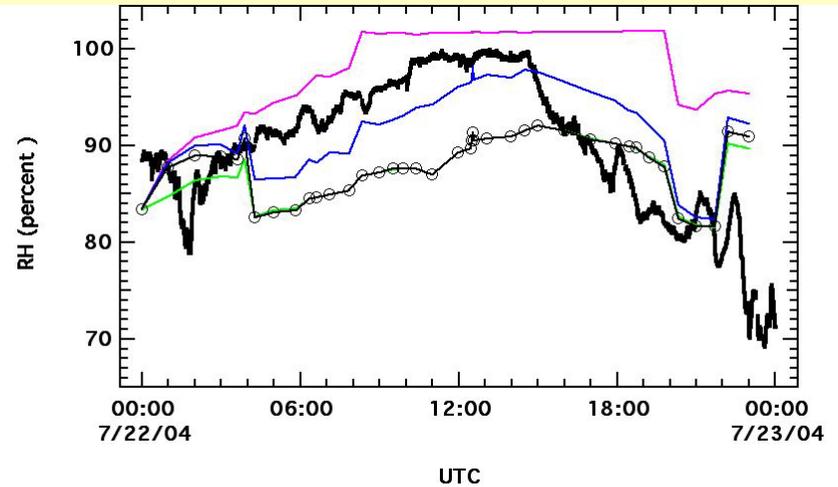
# Comparison with RB Ship Obs. During ICARTT : RH & Wspd

Jul/21/04

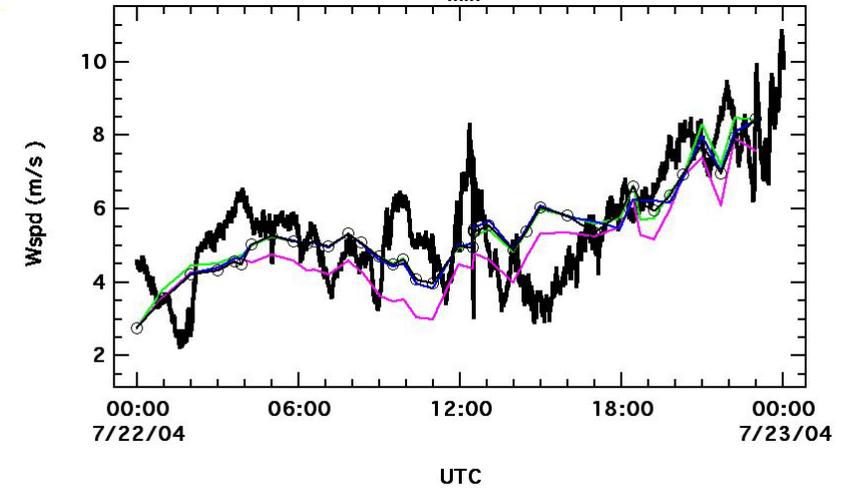
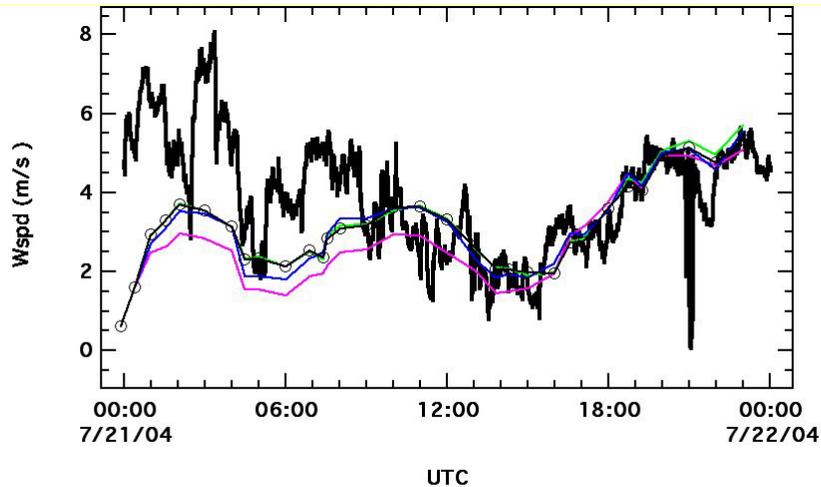


— Observed      — Control  
○—○ Ric=0.5 &  $K_{min}=1$  (m<sup>2</sup>s<sup>-1</sup>) for stable BL

Jul/22/04

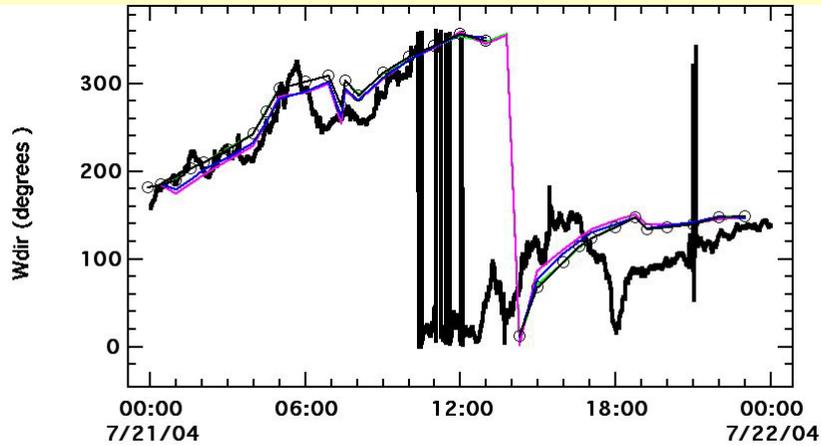


— Ric=0.5 for stable BL  
— Ric=0.5 for stable BL &  $K_{min}=1$  (m<sup>2</sup>s<sup>-1</sup>) for all stability



# Comparison with RB Ship Obs. During ICARTT : **Wdir**

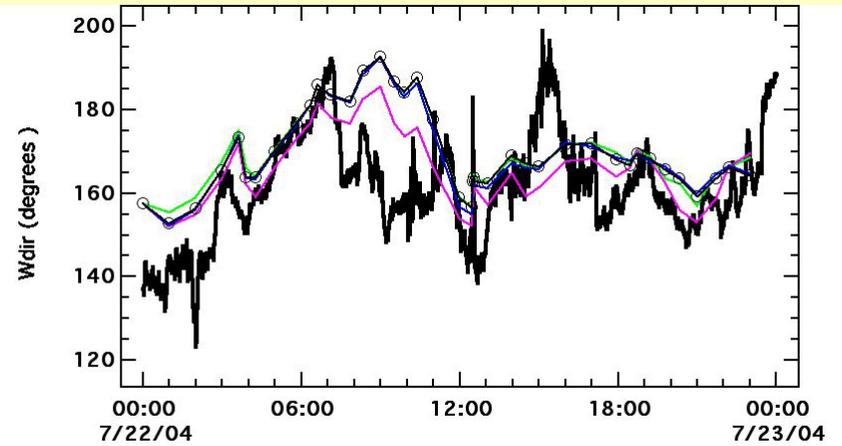
Jul/21/04



UTC

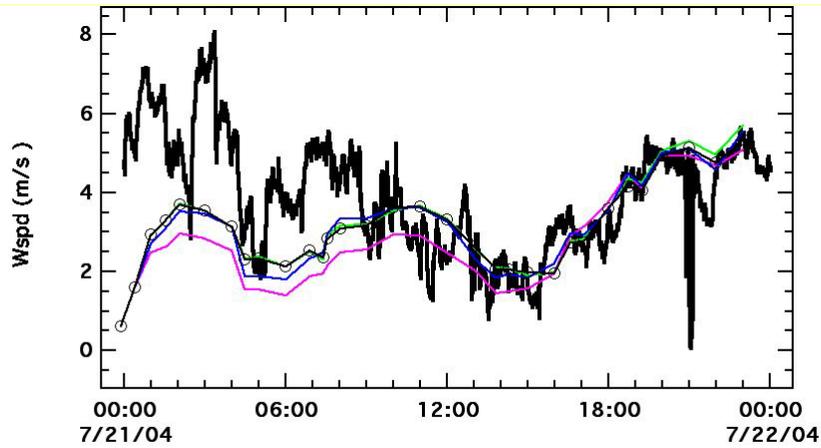
— Observed  
—○— Ric=0.5 &  $K_{min}=1$  ( $m^2s^{-1}$ ) for stable BL  
— Control

Jul/22/04

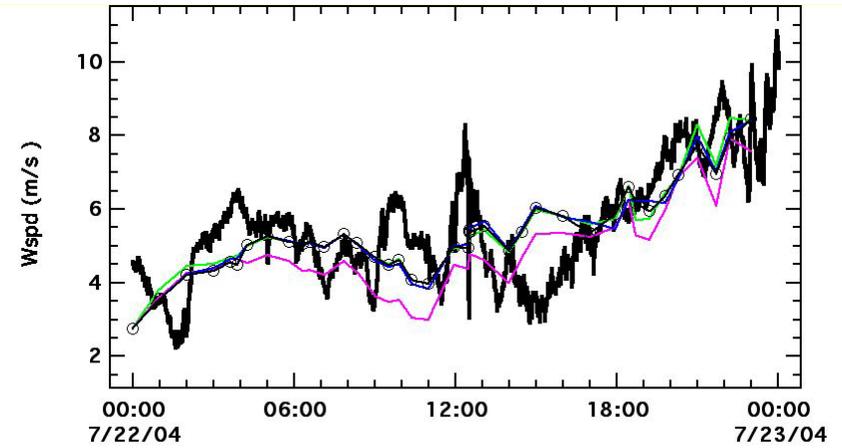


UTC

— Ric=0.5 for stable BL  
— Ric=0.5 for stable BL &  $K_{min}=1$  ( $m^2s^{-1}$ ) for all stability  
— Control



UTC

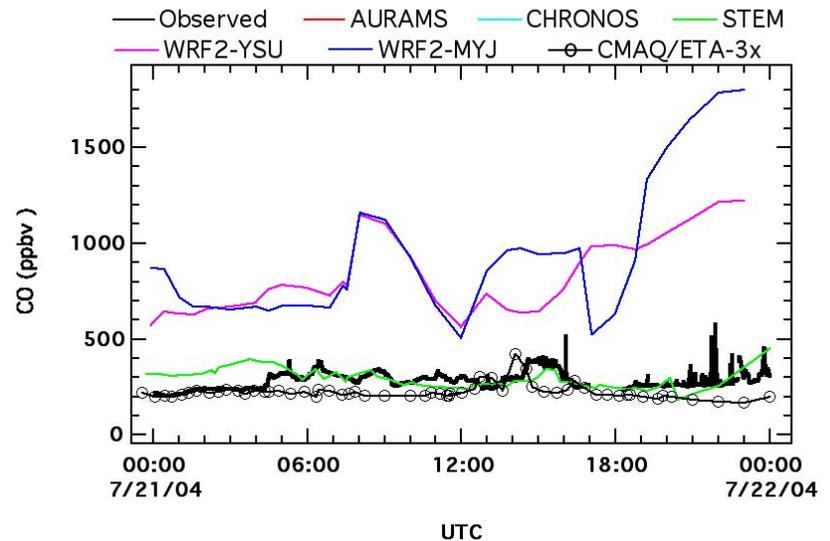
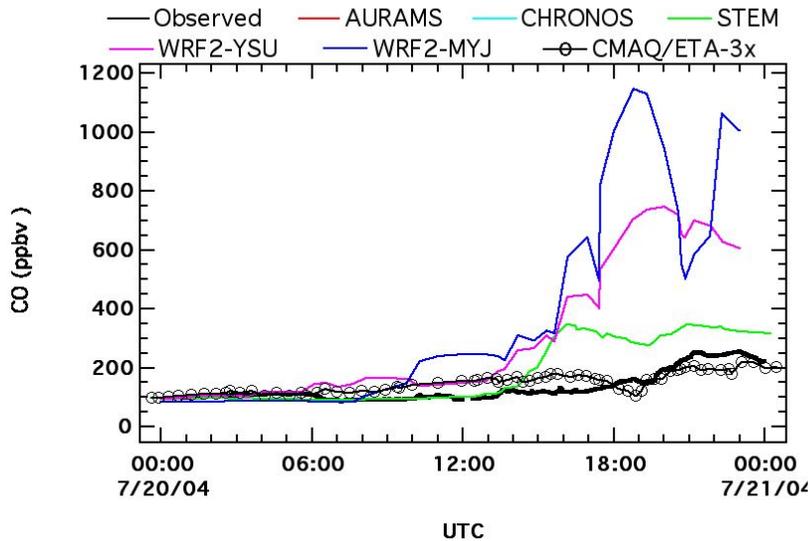
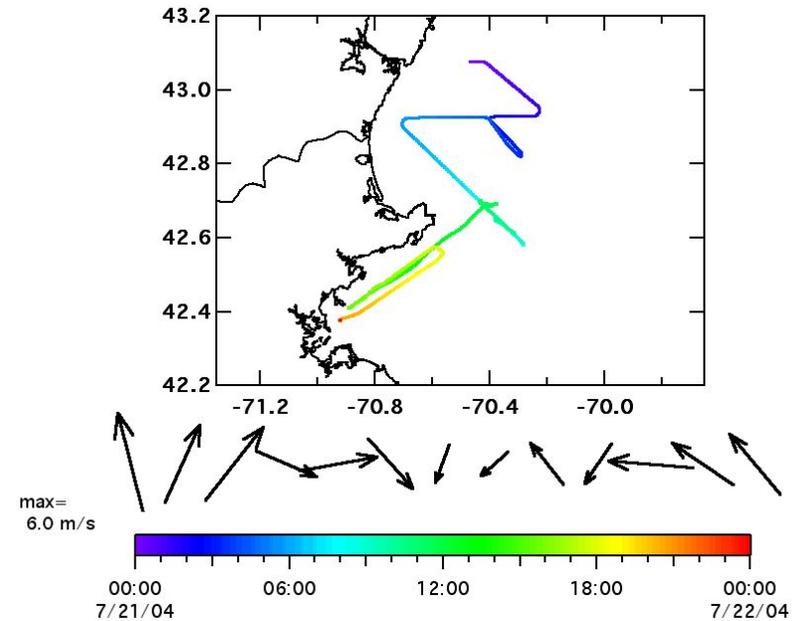
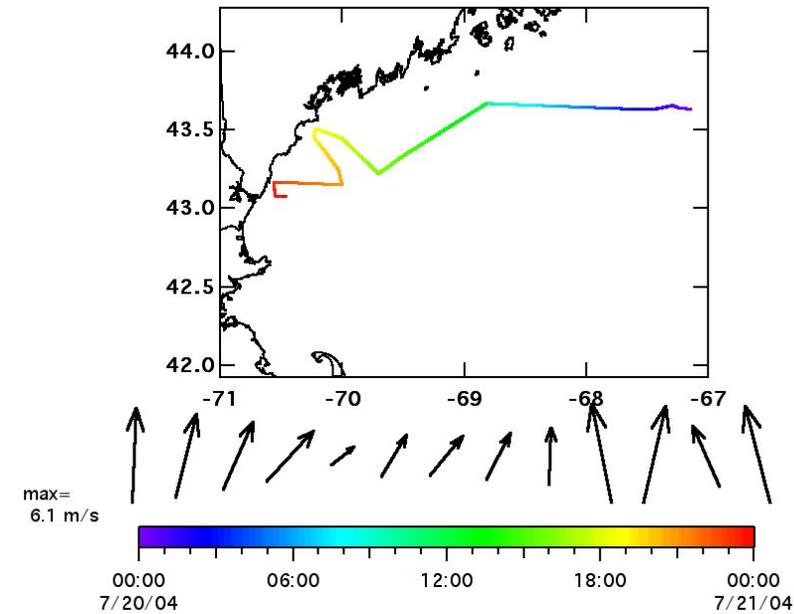


UTC

# YSU vs. MYJ

Jul/20/04

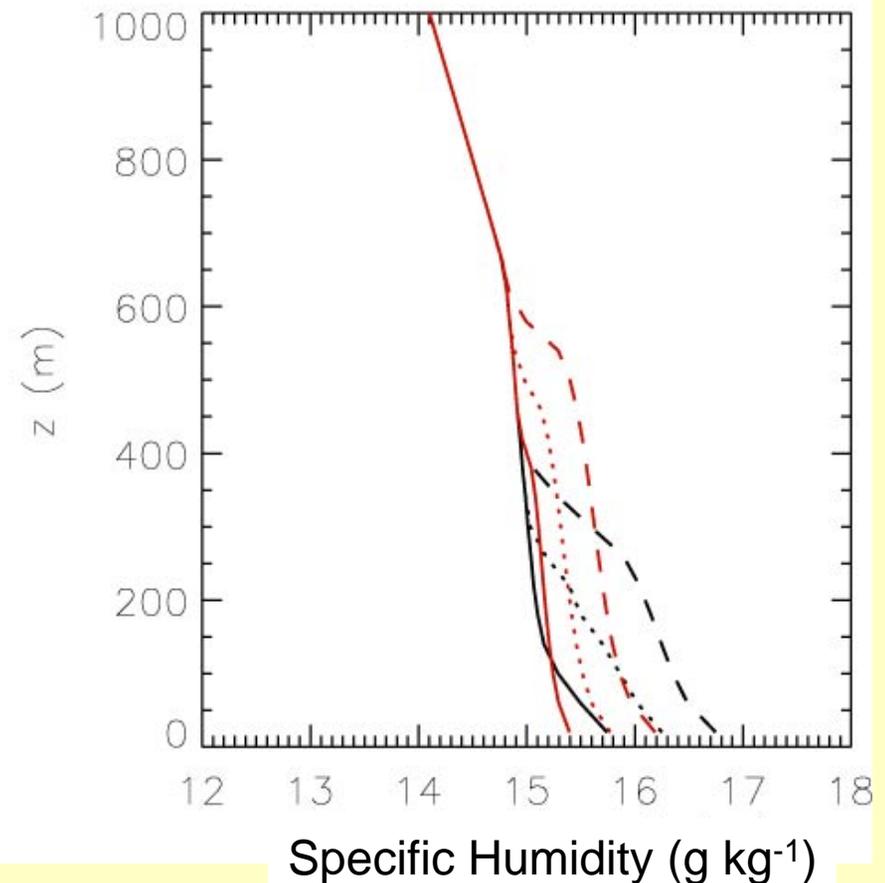
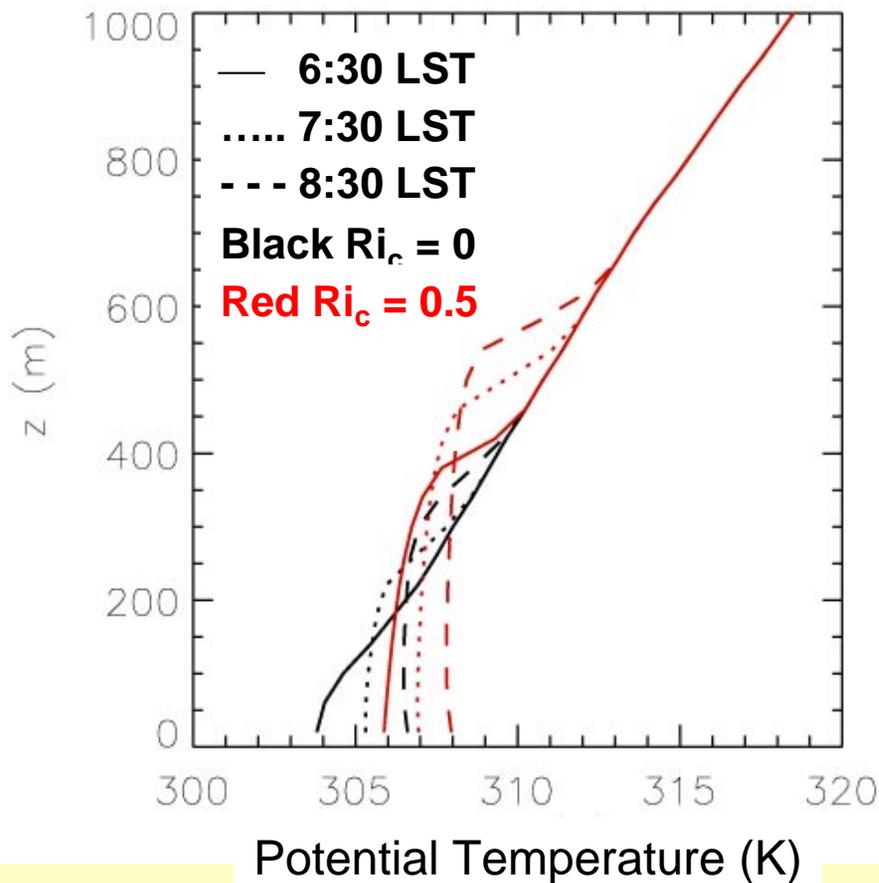
Jul/21/04



# Changing stable BL representation in YSU : $Ri_c$ , $K_z$

Example) Application of a column model to ARM case

Initialized at 5:30 LST, June 21, 1997, SGP



# Vertical profile of model NO<sub>2</sub> and K over water : YSU

