

# UNDERSTANDING THE ROLE OF TURBULENCE ON IN-CANOPY CHEMISTRY AT THE PROPHET SITE

**Sarah C. Kavassalis<sup>1</sup>,**  
Jennifer G. Murphy<sup>1</sup>,  
Allison L. Steiner<sup>2</sup>

<sup>1</sup> Department of  
Chemistry, University of  
Toronto

<sup>2</sup> Climate and Space  
Science and Engineering,  
University of Michigan

September 13<sup>th</sup>, 2017  
*6th Annual IACPES  
Symposium on  
Atmospheric Chemistry  
and Physics*

# ACKNOWLEDGEMENTS

- **Jennifer Murphy**
- **Allison Steiner**
- **Dylan Millet**
- **Hari Alwe**
- **Phil Stevens**
- **Steve Bertman**
- **Chris Vogel (AmeriFlux)**
- The Murphy and Steiner groups
- The PROPHET-AMOS team

AN NSERC CREATE PROGRAM

# IACPES

INTEGRATING ATMOSPHERIC CHEMISTRY AND PHYSICS  
FROM EARTH TO SPACE



UNIVERSITY of TORONTO

THE CENTRE FOR GLOBAL CHANGE SCIENCE

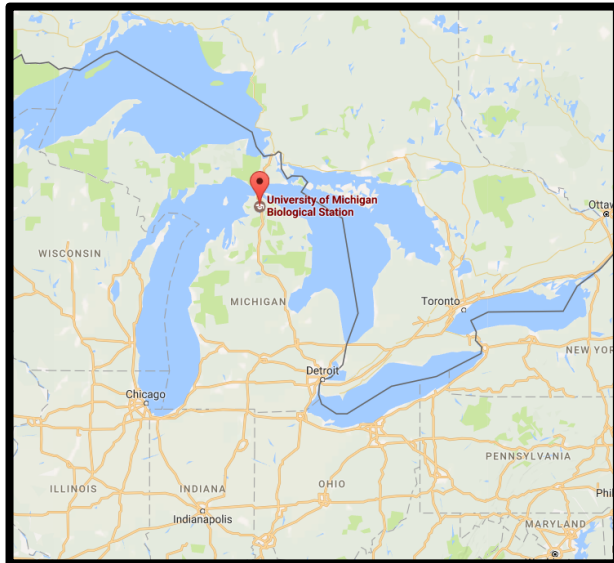




# PROPHET-AMOS CAMPAIGN

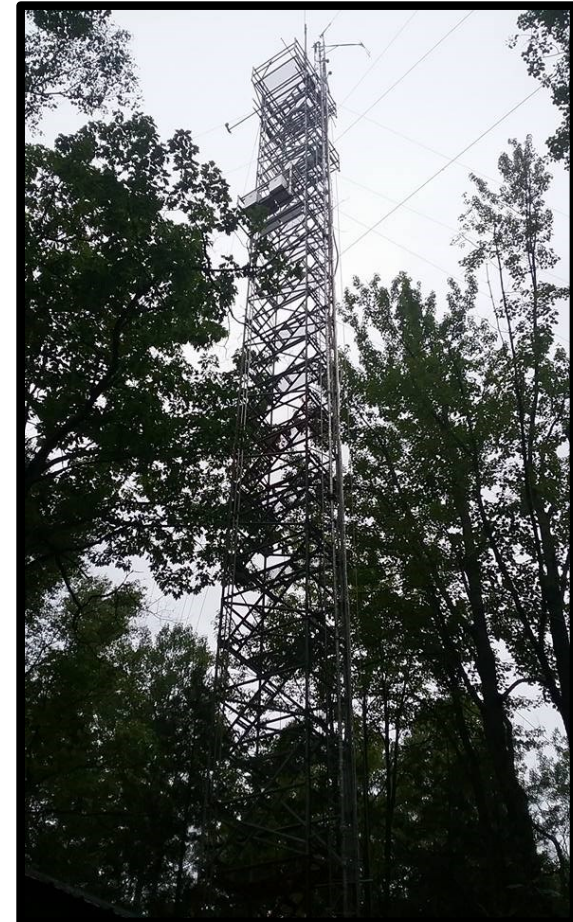
July 1<sup>st</sup> – 31<sup>st</sup>, 2016

University of  
Michigan Biological  
Station



- 22-institute collaboration
- Temperate-Boreal transition forest (mixed wood)
- Average LAI 3.3  $\text{m}^2/\text{m}^2$
- Site houses two flux towers (PROPHET 34m, AmeriFlux 46m) and one lab

**Campaign Goal: Improve our understanding of radical chemistry in forested environments**



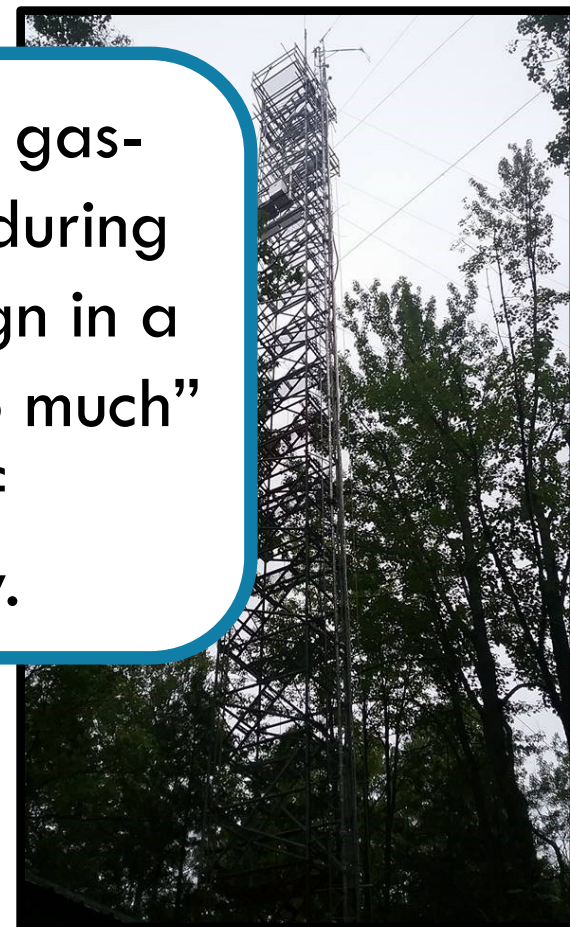
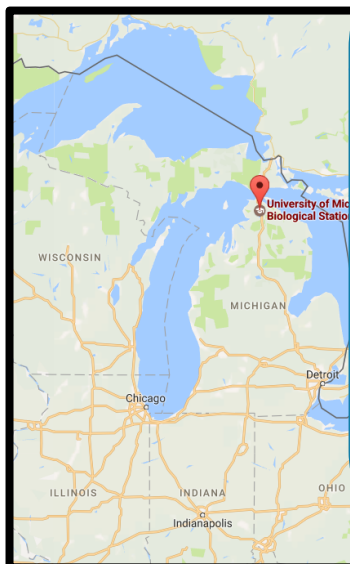
# PROPHET-AMOS CAMPAIGN

July 1<sup>st</sup> – 31<sup>st</sup>, 2016

University of  
Michigan Biological  
Station

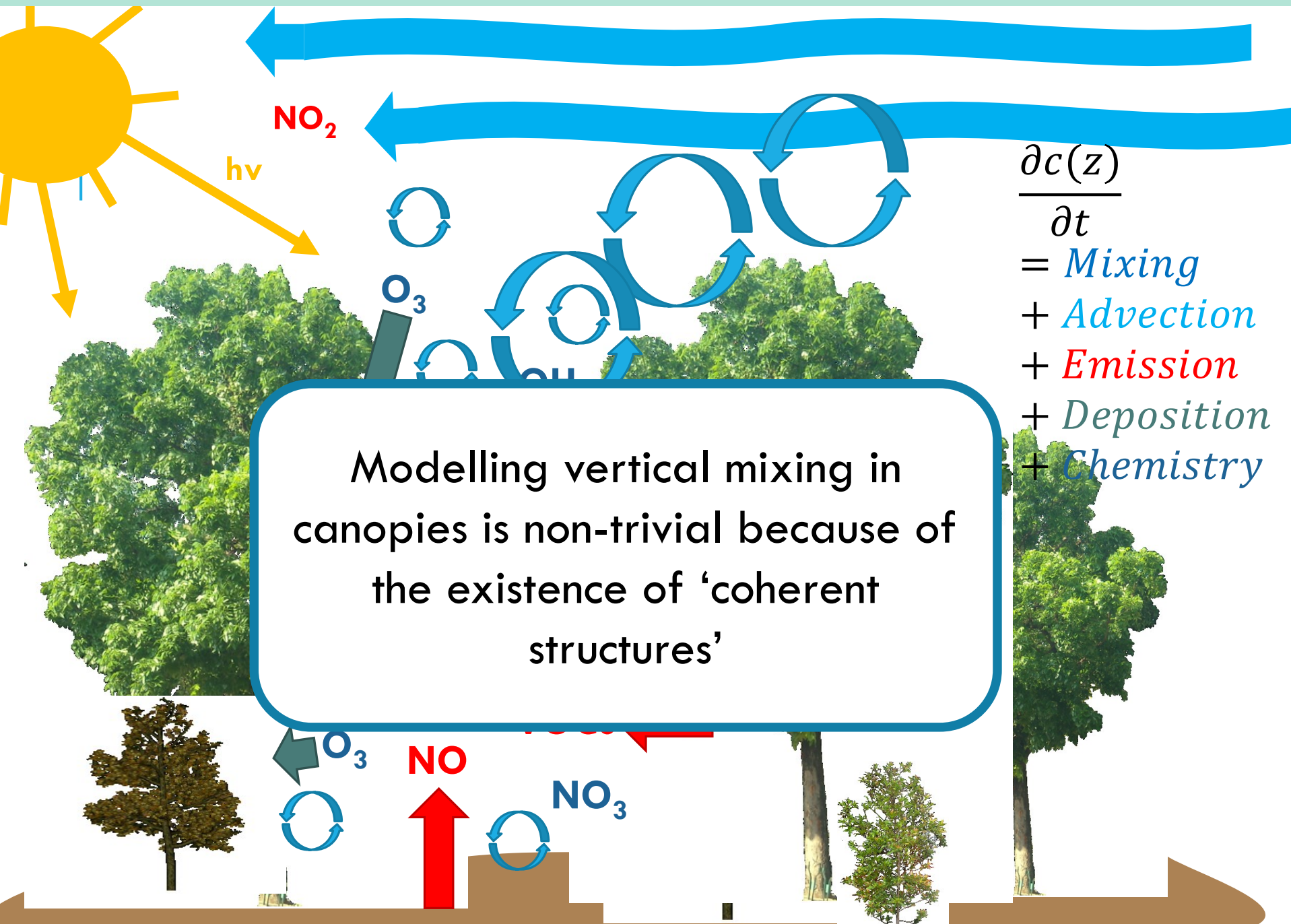
- 22-institute collaboration
- Temperate-Boreal

Goals of this project: Model gas-phase chemistry and mixing during the PROPHET-AMOS campaign in a way that doesn't sacrifice "too much" accuracy in the name of computational efficiency.



**Campaign Goal: Improve our understanding of radical chemistry in forested environments**

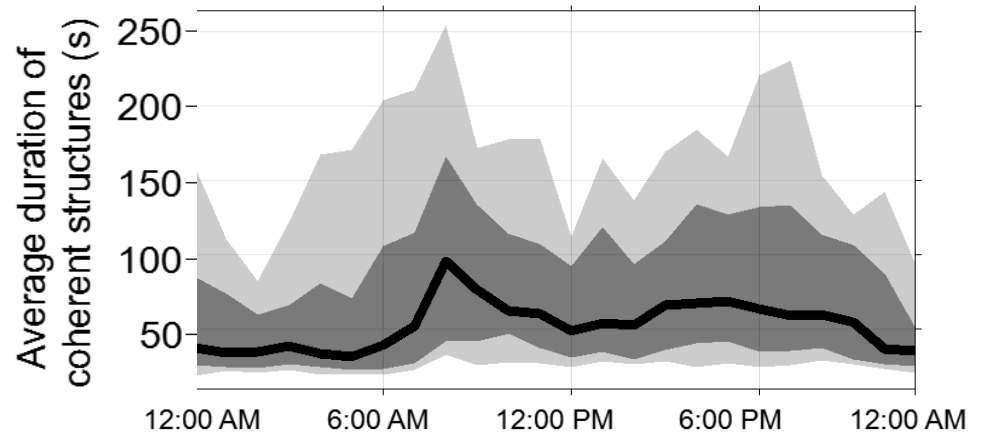
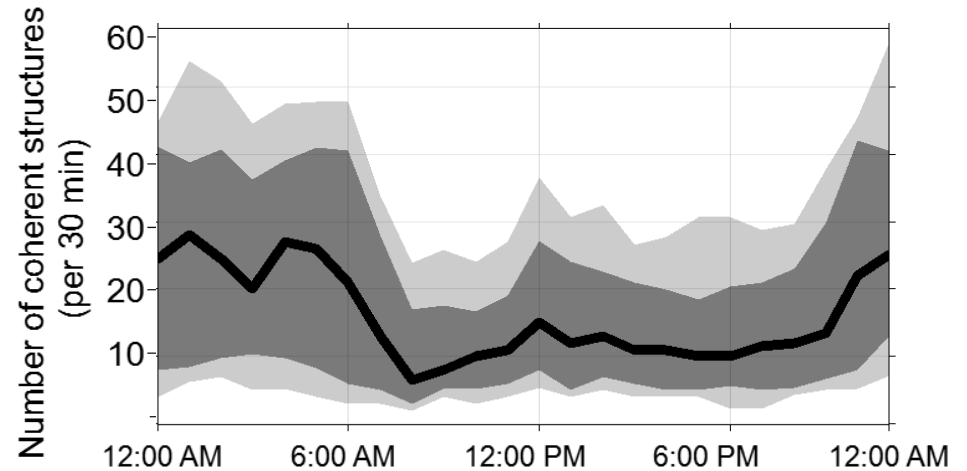
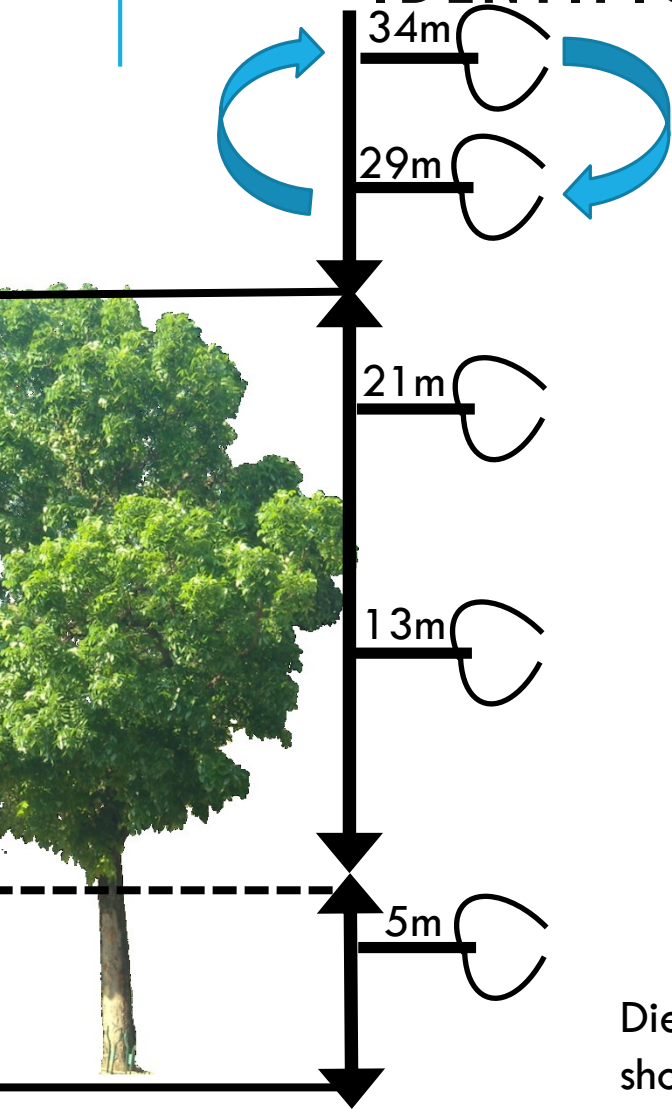




Modelling vertical mixing in canopies is non-trivial because of the existence of 'coherent structures'

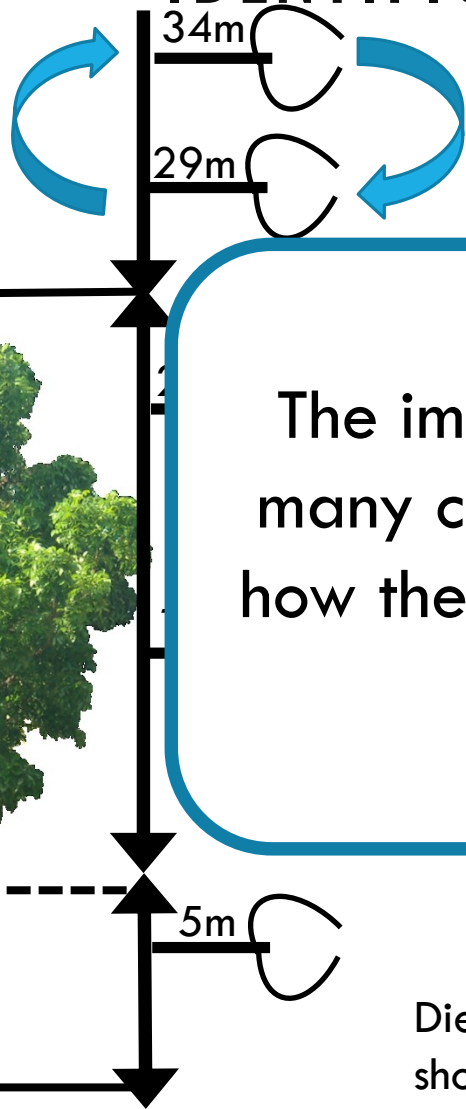
$$\frac{\partial c(z)}{\partial t} = \text{Mixing} + \text{Advection} + \text{Emission} + \text{Deposition} + \text{Chemistry}$$

# IDENTIFICATION OF COHERENT STRUCTURES

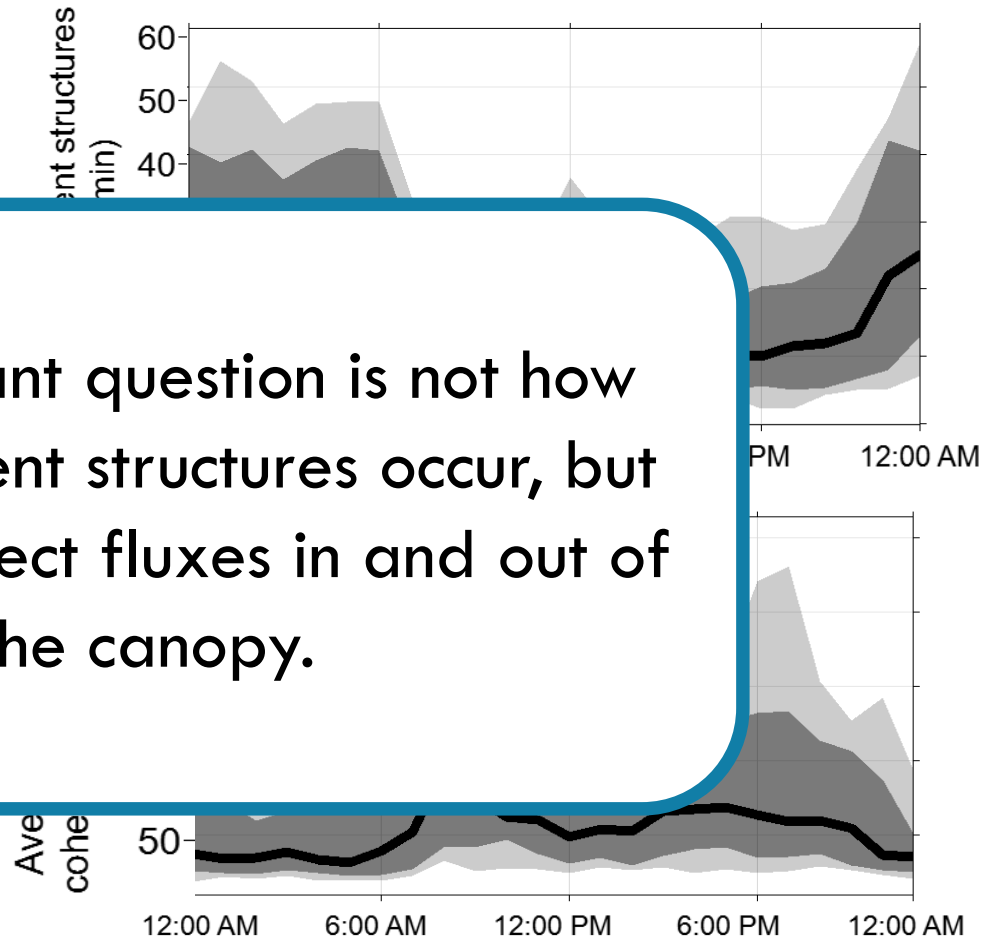


Diel plots of the number and average duration of coherent (s) showing campaign median, 25<sup>th</sup>/75<sup>th</sup>, and 5<sup>th</sup>/95<sup>th</sup> quantiles.

# IDENTIFICATION OF COHERENT STRUCTURES

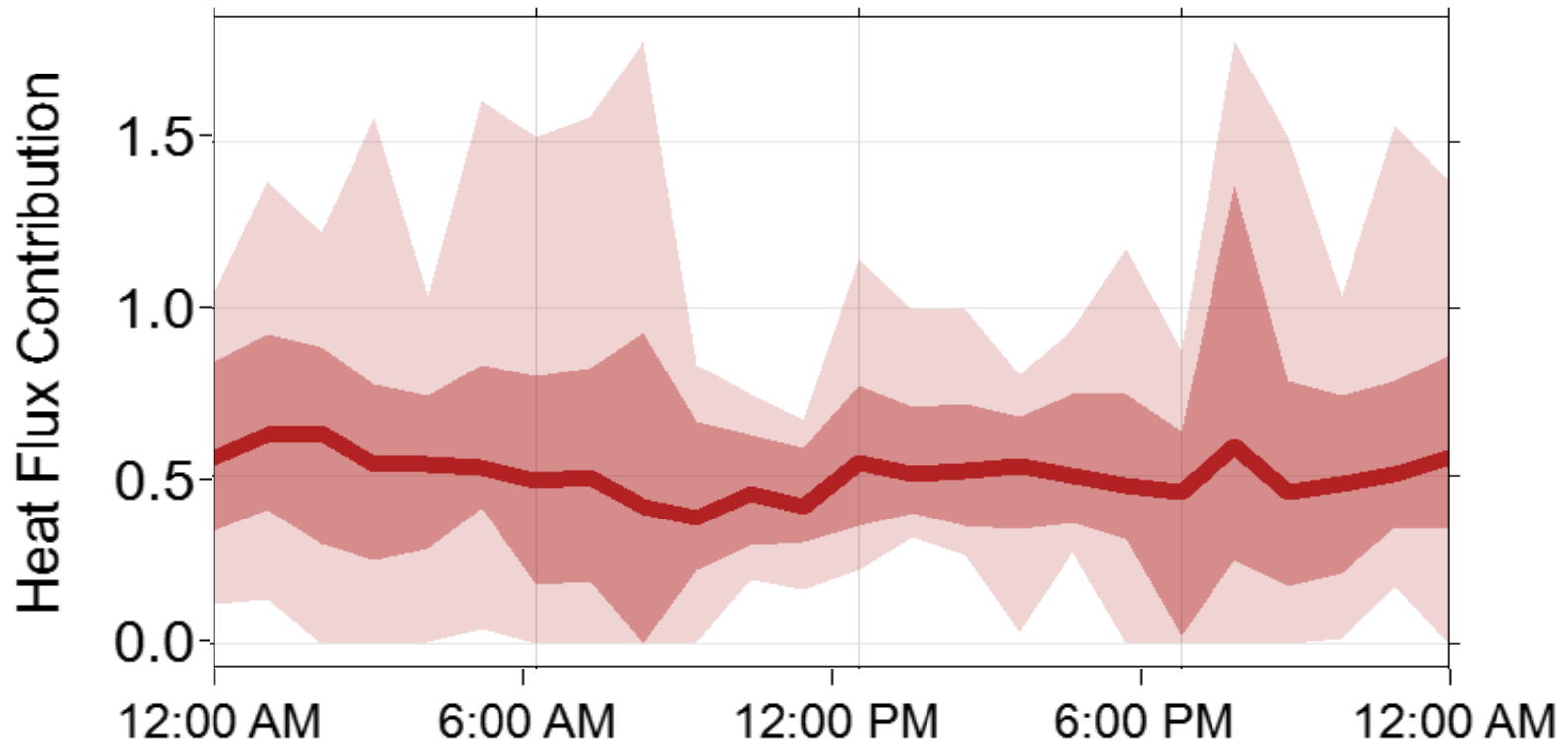


The important question is not how many coherent structures occur, but how they affect fluxes in and out of the canopy.



Diel plots of the number and average duration of coherent (s) showing campaign median, 25<sup>th</sup>/75<sup>th</sup>, and 5<sup>th</sup>/95<sup>th</sup> quantiles.

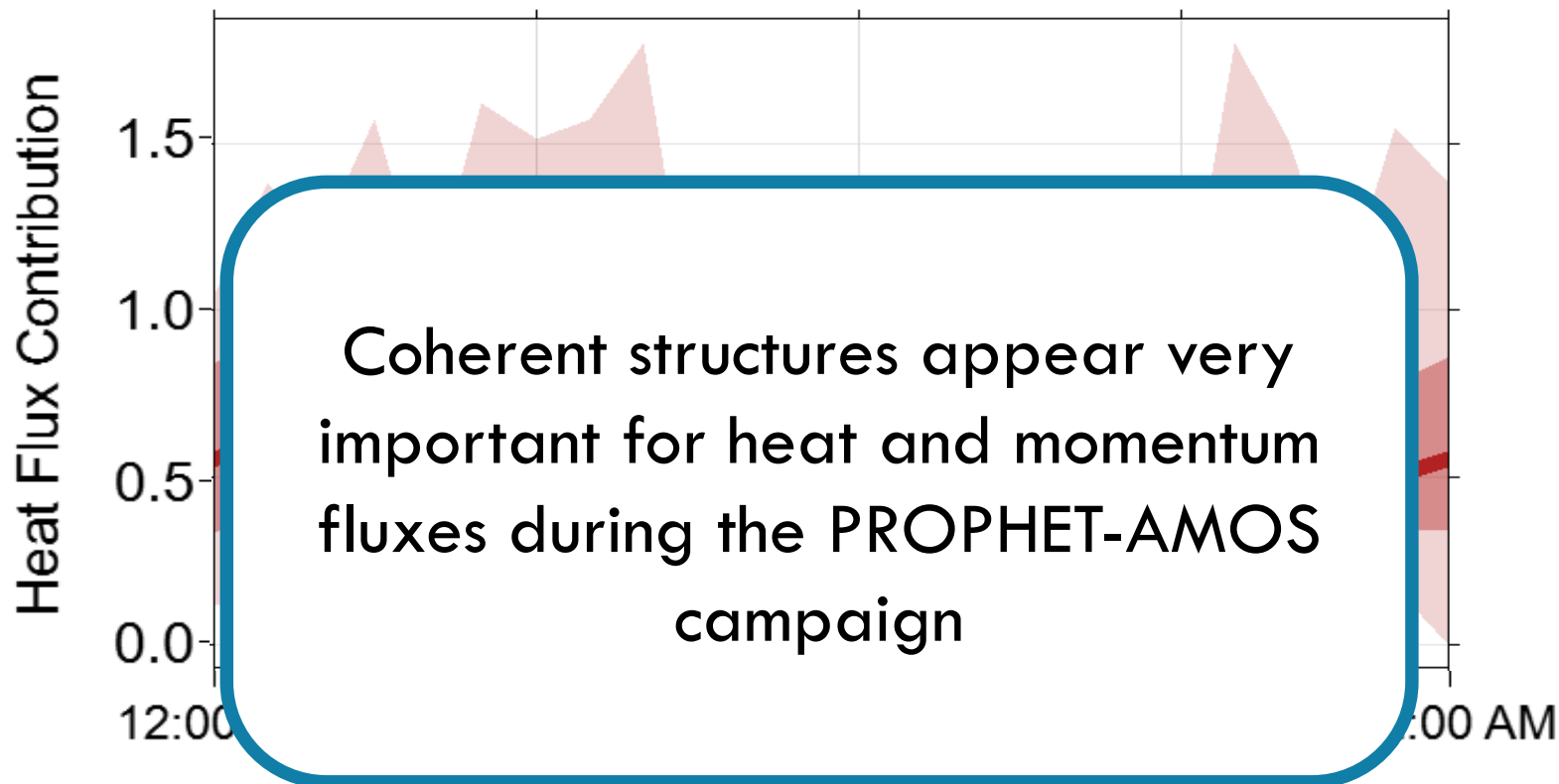
# IMPORTANCE OF COHERENT STRUCTURES



Diel plot of the fractional contribution of coherent structures to kinematic heat flux showing campaign median, 25<sup>th</sup>/75<sup>th</sup>, and 5<sup>th</sup>/95<sup>th</sup> quantiles.



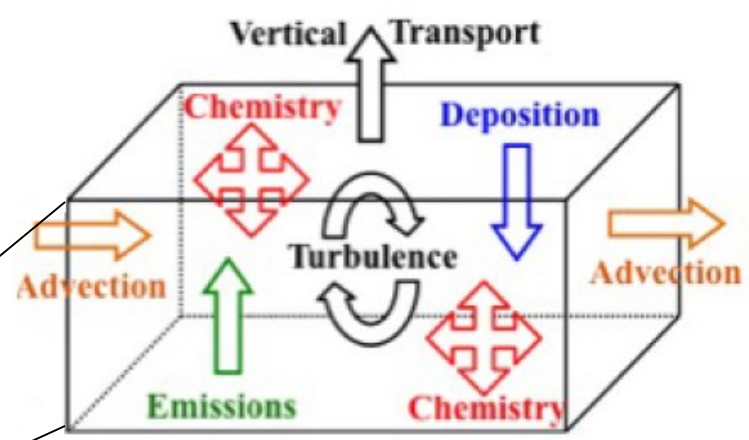
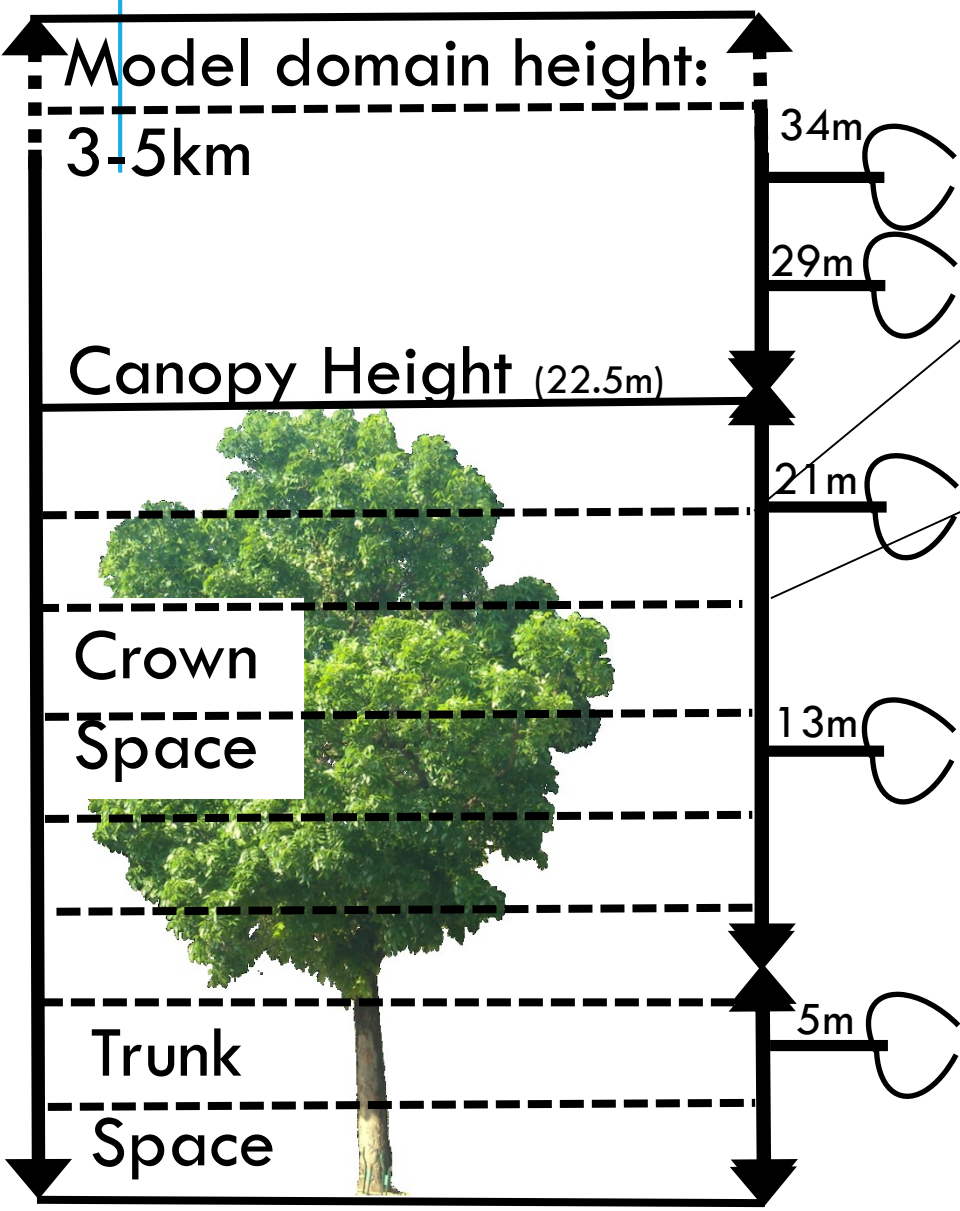
# IMPORTANCE OF COHERENT STRUCTURES



Diel plot of the fractional contribution of coherent structures to kinematic heat flux showing campaign median, 25<sup>th</sup>/75<sup>th</sup>, and 5<sup>th</sup>/95<sup>th</sup> quantiles.

# THE FORCAST MODEL

Forkel et al., 2006.  
 Bryan et al., 2012.  
 Ashworth et al., 2015.



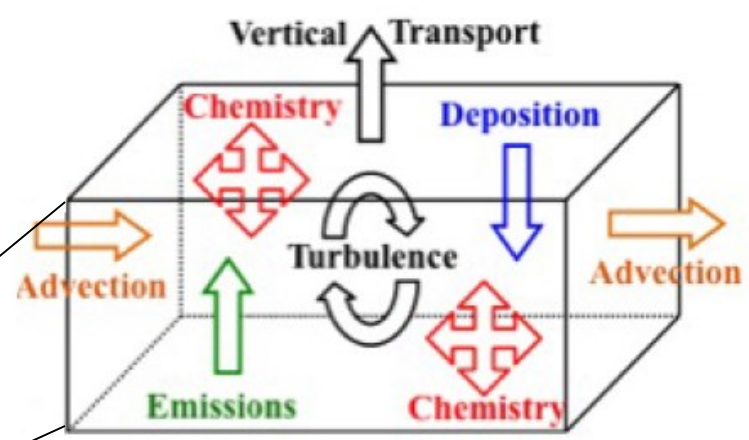
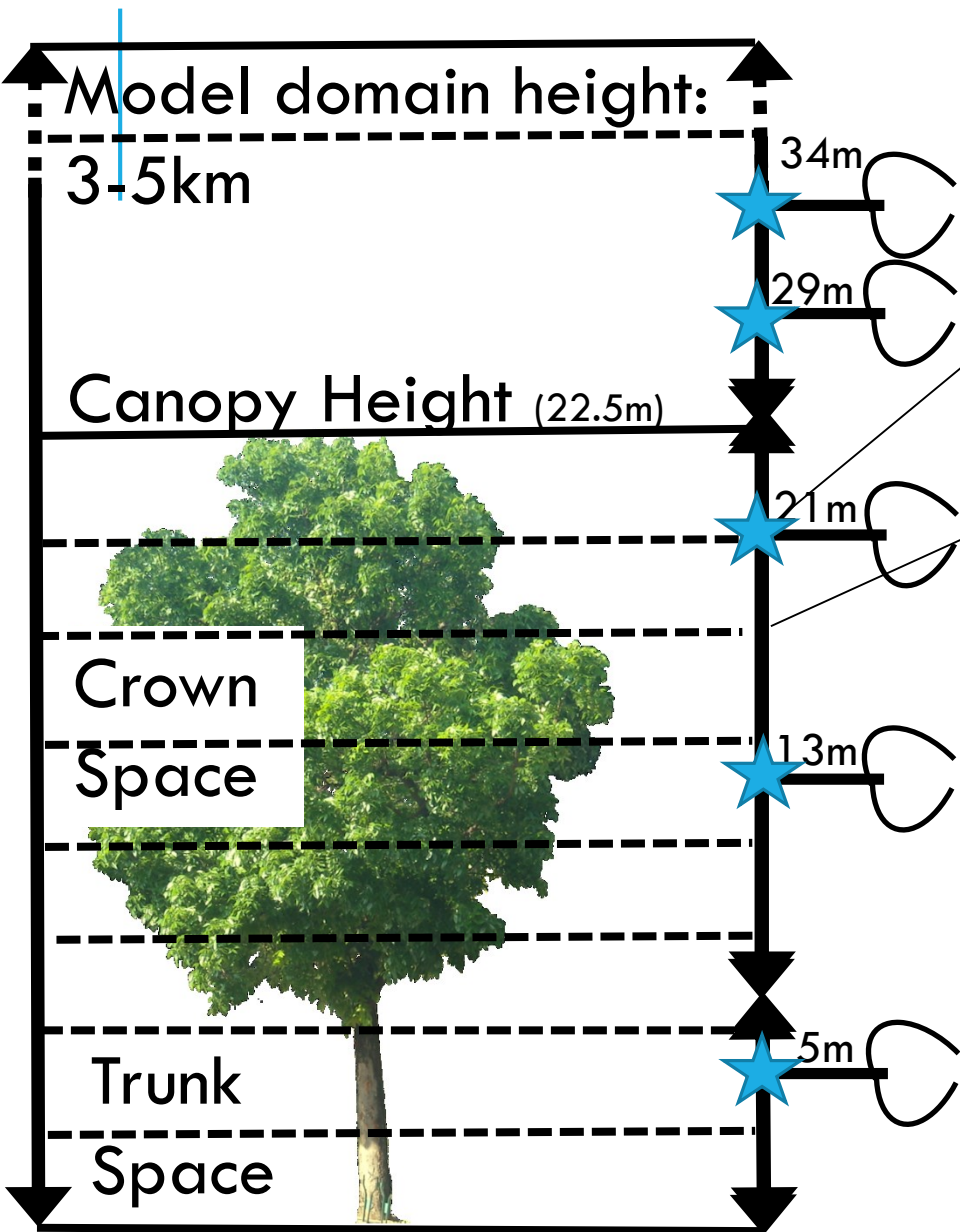
FORCAsT (Ashworth et al., 2015) was constrained by PROPHET-AMOS observations and used to model the campaign chemistry. In FORCAsT, mass fluxes are calculated by solving the continuity equation:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z} \left( K_H \frac{\partial c}{\partial z} \right) + S_c + C$$

Where  $c$  is the mixing ratio of the species of interest,  $K_H$  is the turbulence exchange coefficient,  $S_c$  includes contributions from emissions, deposition, and advection, and  $C$  represents chemical production and loss.

# THE FORECAST MODEL

Forkel et al., 2006.  
 Bryan et al., 2012.  
 Ashworth et al., 2015.



We define and observed  $K_H$  following Makar et al. (1999)

$$K_{H,obs} = \sigma_w^2 \frac{0.3h}{u_*}$$

Where  $h$  is the height,  $u_*$  is the friction velocity, and  $\sigma_w$  is the standard deviation of the vertical velocity.



# TWO MAJOR QUESTIONS

- 1) How much faith should we put into a 1D canopy model that does not explicitly represent coherent structures?
- 2) How important are sub-canopy constraints on our mixing scheme for modelling chemical mixing ratios?

# HOW WELL CAN WE MODEL CANOPY EXCHANGE WITHOUT EXPLICIT COHERENT STRUCTURES?

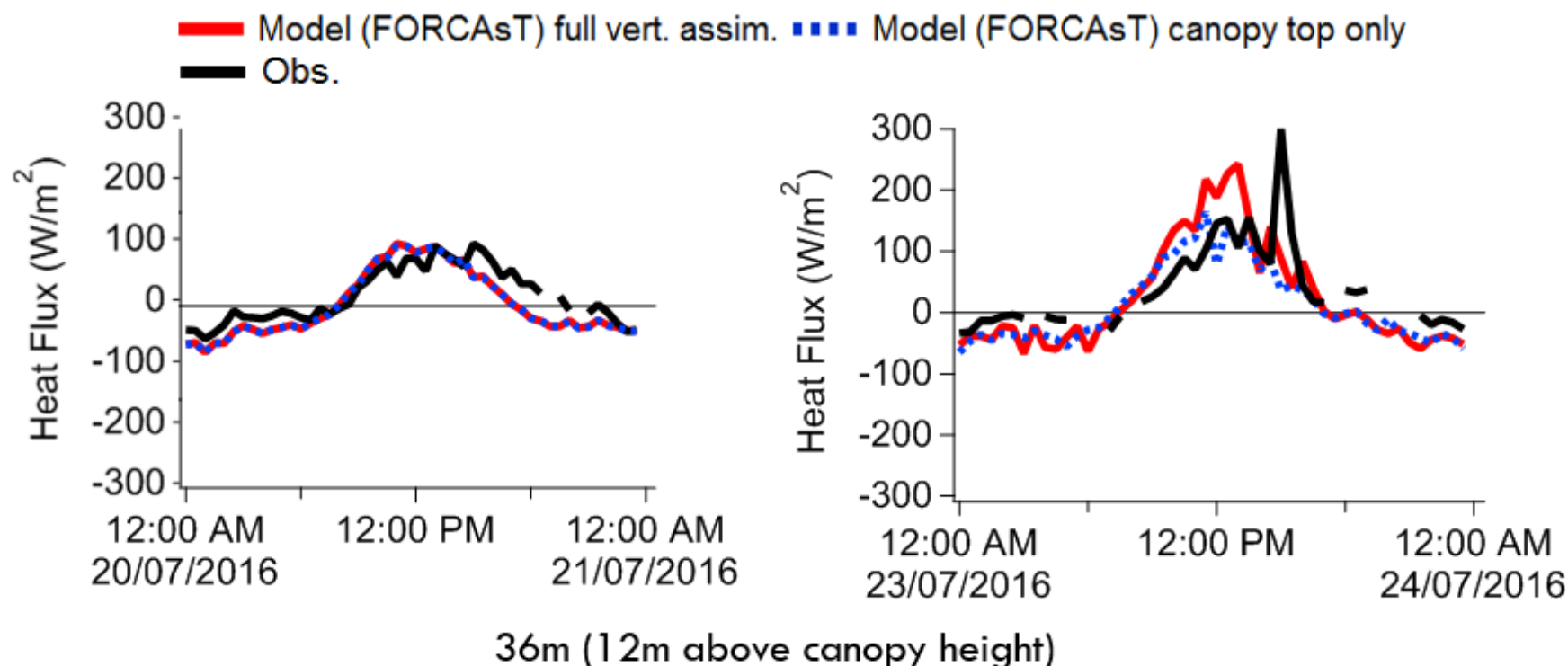
July 20<sup>th</sup>, 2016

Fraction of heat flux attributable to coherent structures = **0.45**

**Campaign average**  
**0.52±0.07**

July 23<sup>rd</sup>, 2016

Fraction of heat flux attributable to coherent structures = **0.62**



# HOW WELL CAN WE MODEL CANOPY EXCHANGE WITHOUT EXPLICIT COHERENT STRUCTURES?

July 20<sup>th</sup>, 2016

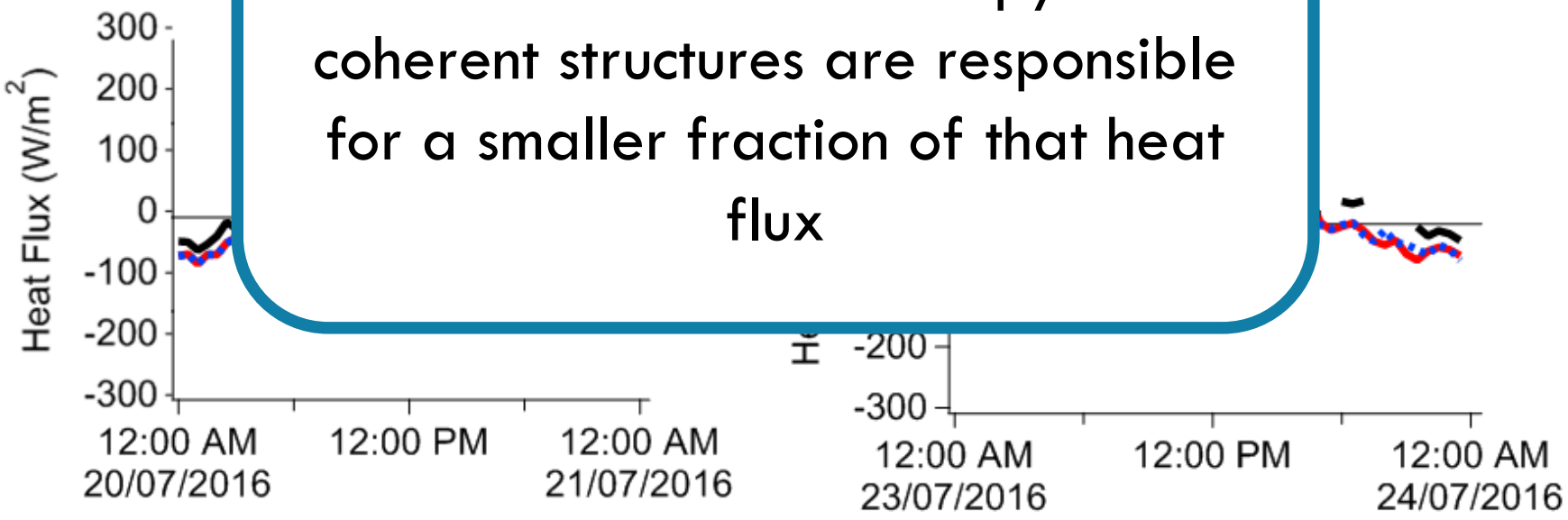
July 23<sup>rd</sup>, 2016

Fraction of heat flux attributed to coherent structures

Campaign

Fraction of heat flux attributed to coherent structures only

We do a better job at modelling heat flux out of the canopy when coherent structures are responsible for a smaller fraction of that heat flux



36m (12m above canopy height)



36m (12m above canopy height)

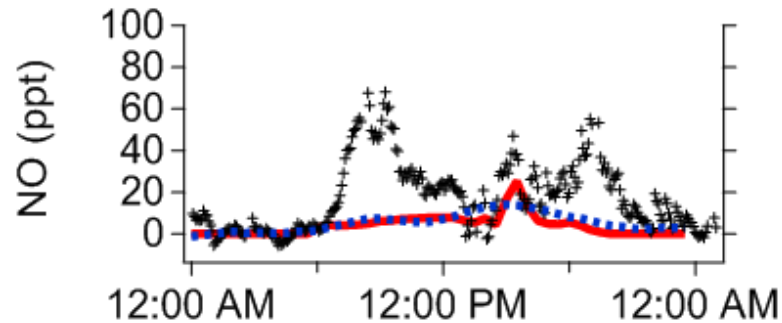
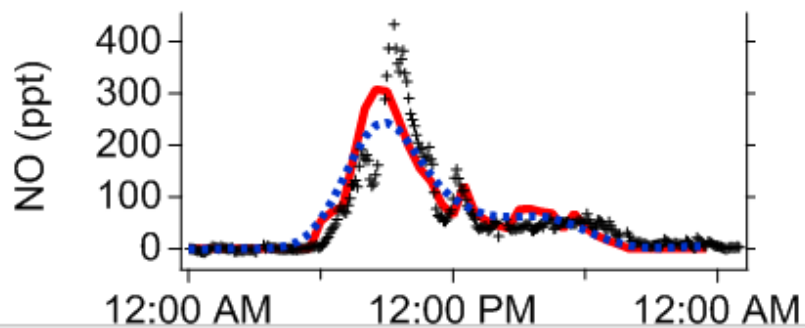
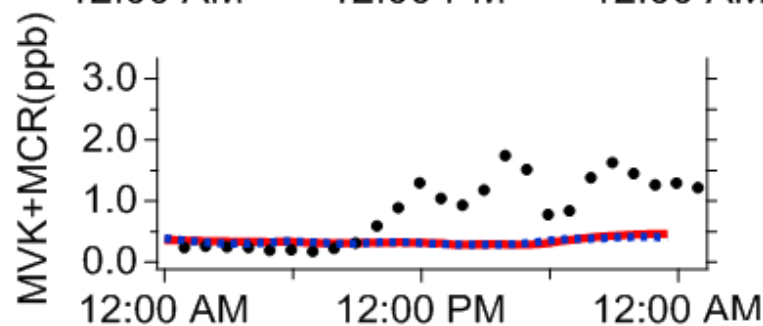
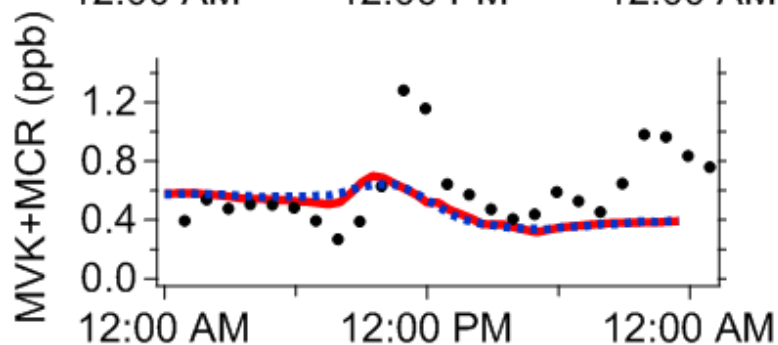
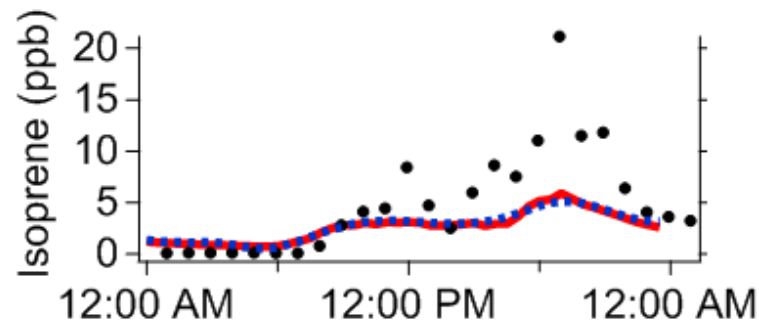
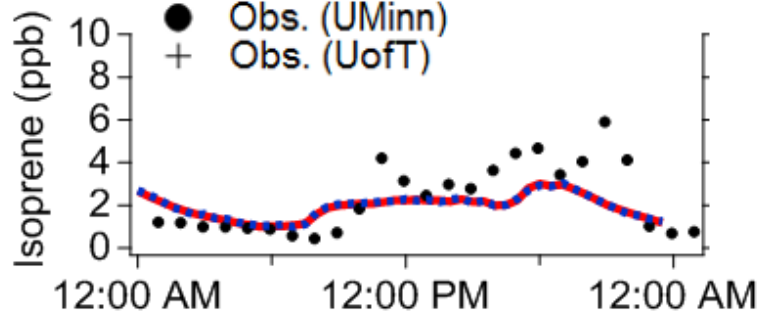
# MODELLING CHEMISTRY DURING PROPHET-AMOS

July 20<sup>th</sup>, 2016

July 23<sup>rd</sup>, 2016

— Model (FORCAsT+CACM) full vert. assim.    - - - Model (FORCAsT+CACM) canopy top only

● Obs. (UMinn)  
+ Obs. (UofT)



# MODELLING CHEMISTRY DURING PROPHET-AMOS

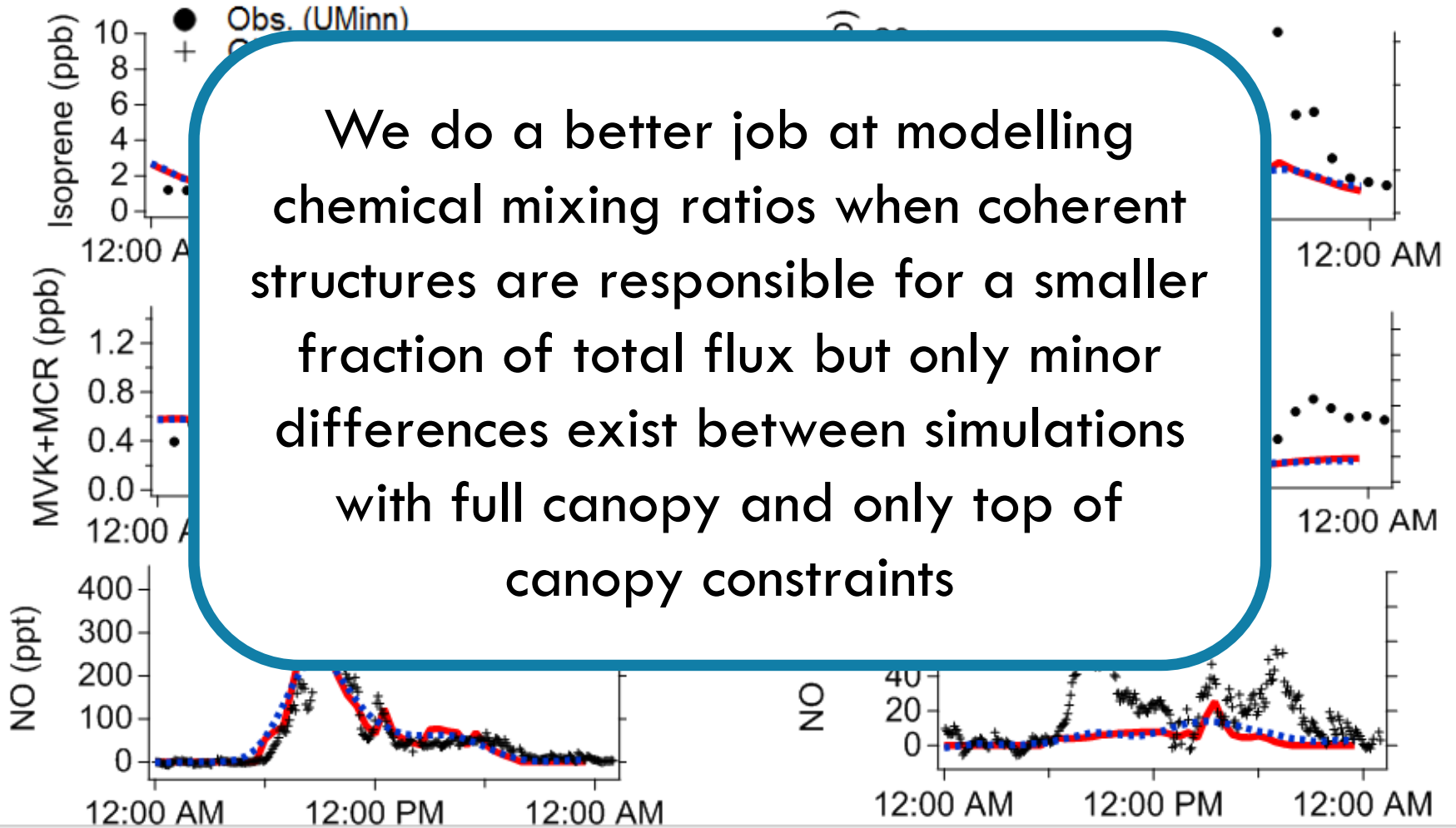
July 20<sup>th</sup>, 2016

July 23<sup>rd</sup>, 2016

— Model (FORCAsT+CACM) full vert. assim.    - - - Model (FORCAsT+CACM) canopy top only

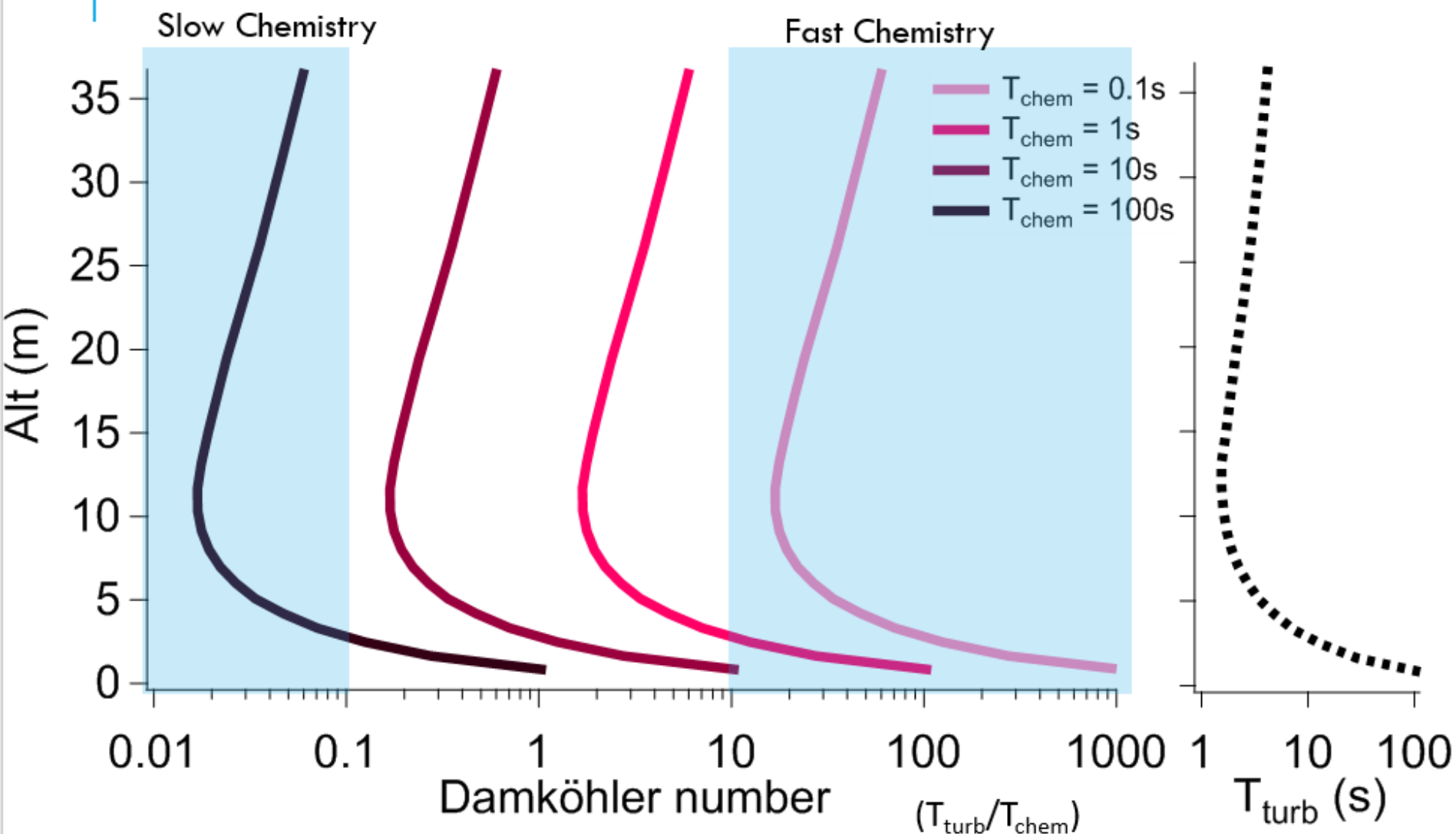
● Obs. (UMinn)

+ Obs. (UMinn)



We do a better job at modelling chemical mixing ratios when coherent structures are responsible for a smaller fraction of total flux but only minor differences exist between simulations with full canopy and only top of canopy constraints

# IMPACT OF TURBULENCE ON CHEMISTRY

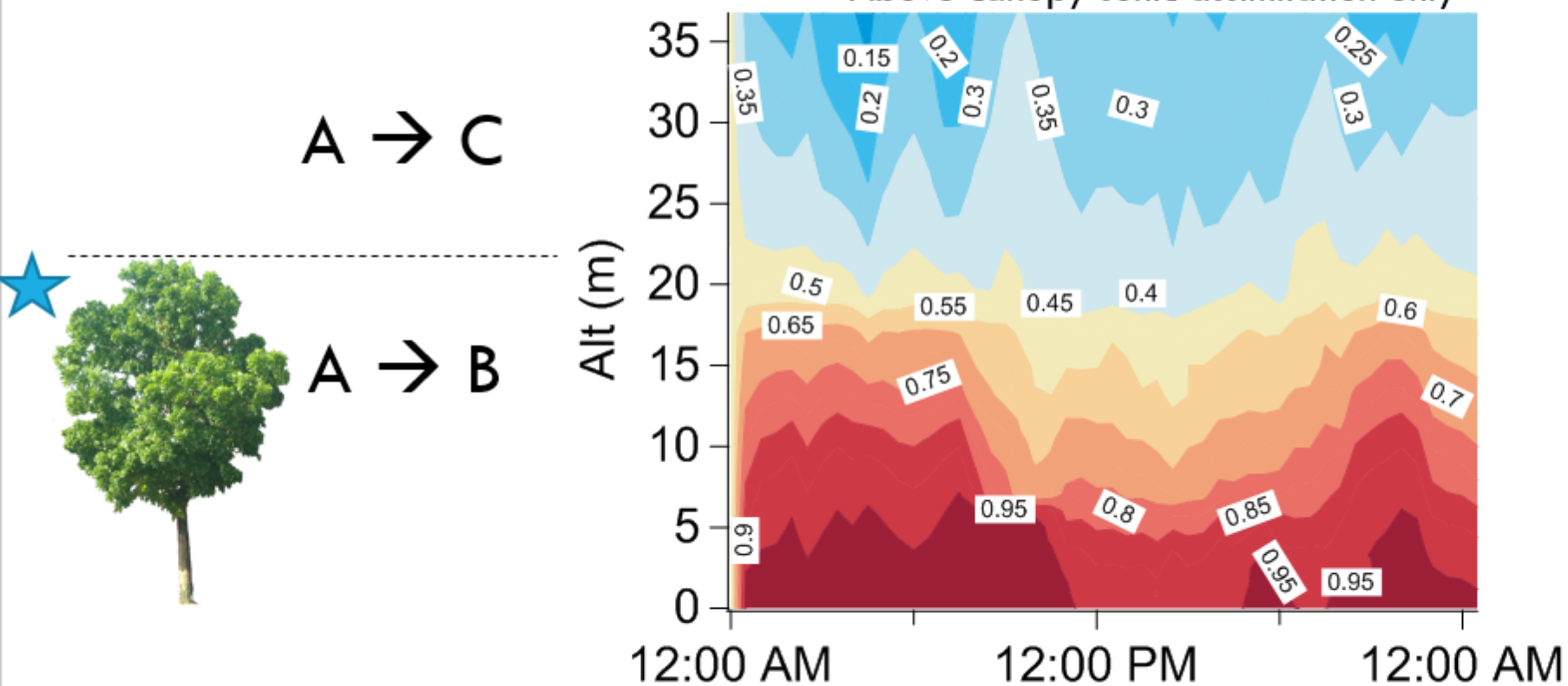




# IMPACT OF TURBULENCE ON CHEMISTRY

Ratio of B to B+C,  $T_{\text{chem}, A} = 0.1\text{s}$

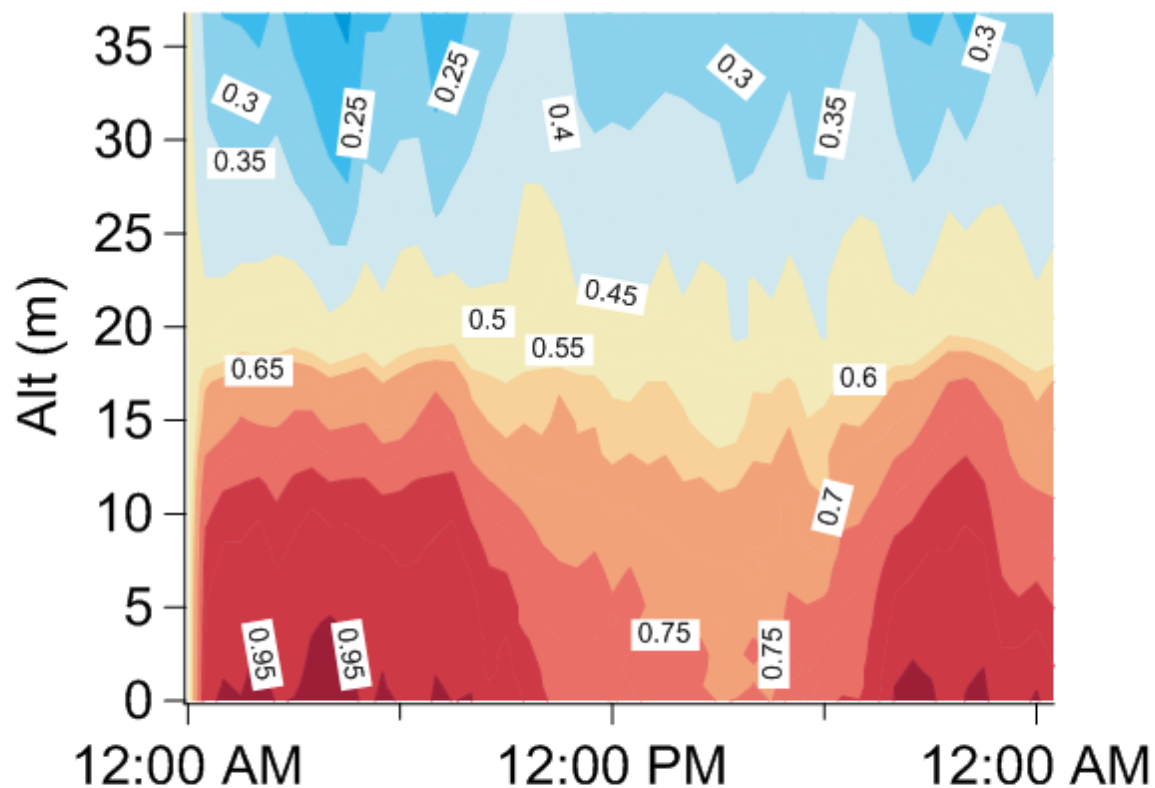
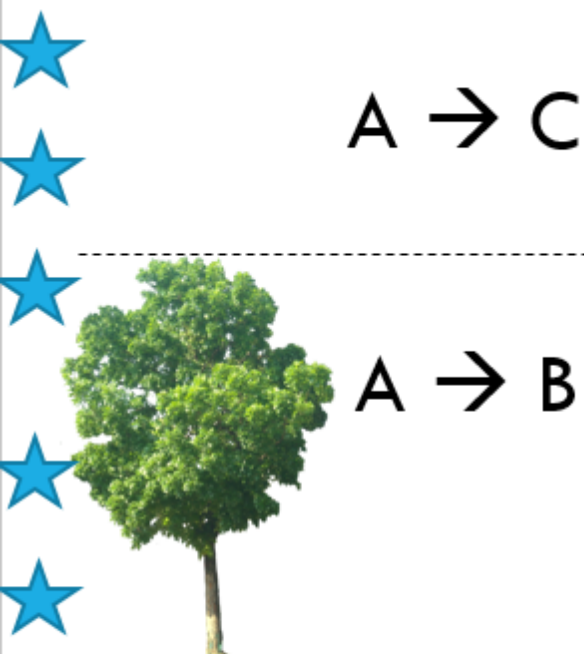
Above canopy sonic assimilation only



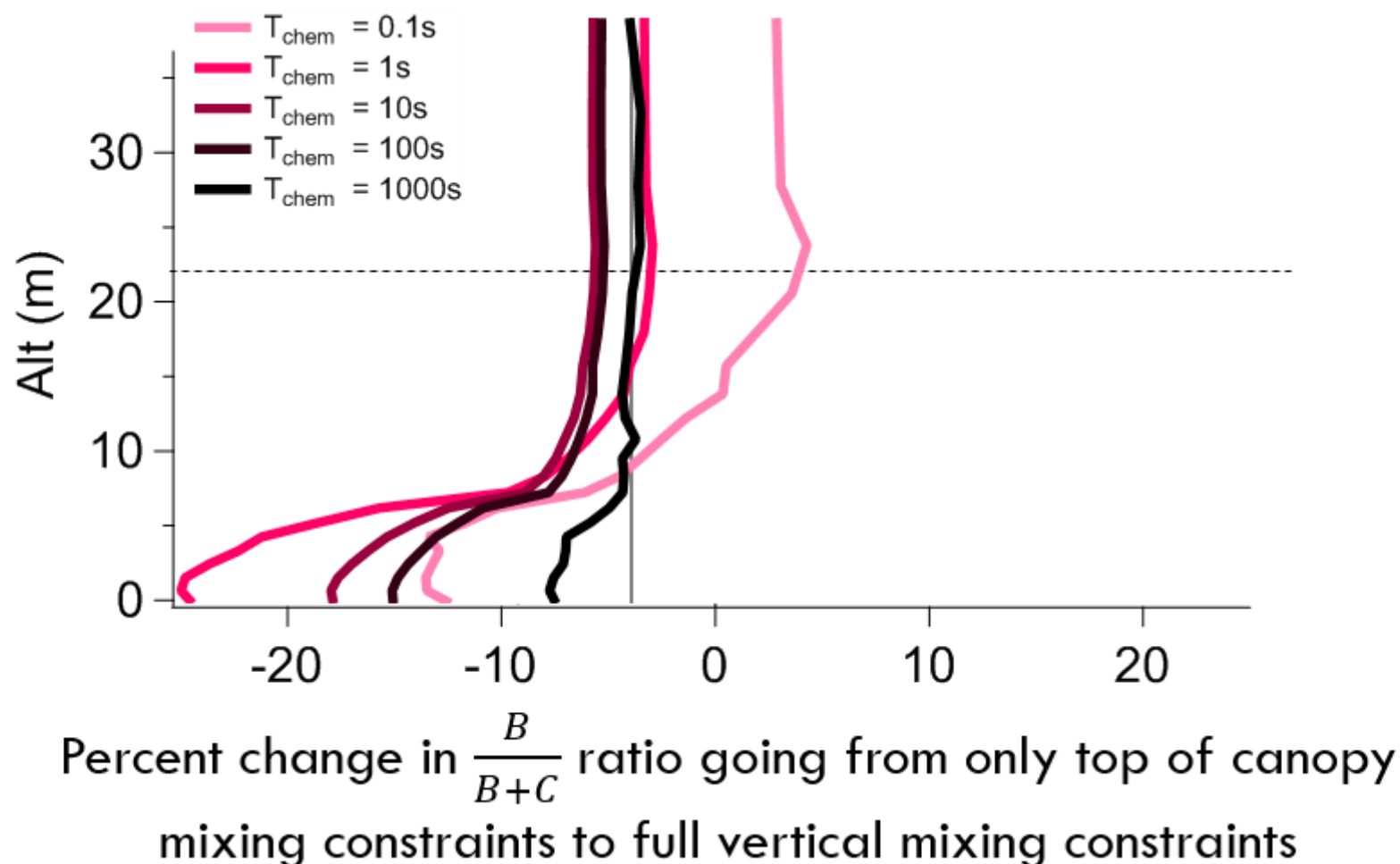
# IMPACT OF TURBULENCE ON CHEMISTRY

Ratio of B to B+C,  $T_{chem, A} = 0.1s$

Full vertical sonic assimilation



# SIGNIFICANCE OF SUBCANOPY CONSTRAINTS ON MIXING



# CONCLUSIONS AND ON-GOING WORK

- We can model heat flux and chemical mixing ratios with reasonable accuracy in a 1D column model without explicit coherent structure representation (despite the large contribution coherent structures make to fluxes) so long as we fix  $K_H$  by observations
- Model preference is best when the fractional contribution of coherent structures to fluxes is the lowest
- Constraining the subcanopy mixing in our model is important for chemical compounds with Damköhler numbers near 1
- By knowing the conditions in which our model recreates vertical exchange the most accurately, we can begin to probe other aspects of the model (like choice of chemical mechanism and dry deposition parametrization)