



# Tropospheric Ozone Production Pathways with Detailed Chemical Mechanisms

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1st July 2015

## Previous Meeting Re-cap

Comparison of  $O_3$  Production in Chemical Mechanisms

Impact of Solvent Speciations on  $O_3$

Sensitivity of  $O_3$  Production on Modelled Conditions

Timeline

# Action Points from Last Meeting

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- ▶ Submit mechanism comparison paper to ACP. ✓
- ▶ Analysis for solvent sector emissions model runs. ✓
- ▶ Modelling work for third paper. **In progress**
- ▶ Action plan timeline for finishing PhD. ✓

Previous Meeting Re-cap

Comparison of  $O_3$  Production in Chemical Mechanisms

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Timeline

- ▶ Submitted to ACP on 10th April.
- ▶ Robert Harley is the editor.
- ▶ Accepted for discussion phase on 13th April.
- ▶ Manuscript appeared in ACPD forum till 8th July.

- ▶ Generally positive review.
- ▶ Commented that the older versions of the mechanisms should be considered as “relics of the past”.
- ▶ Manuscript gives the impression that we consider the MCM to be “correct”.
- ▶ Question on how much we learn about ozone production from more explicit versus less chemical mechanisms.

Previous Meeting Re-cap

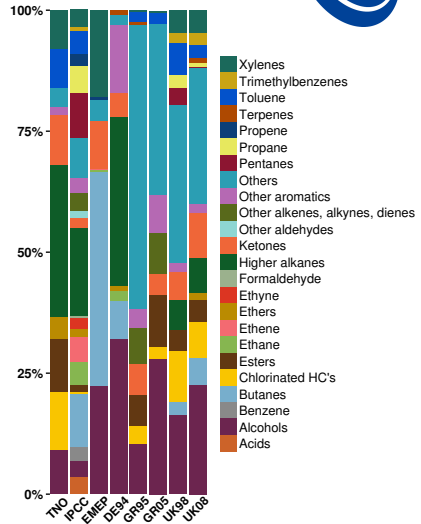
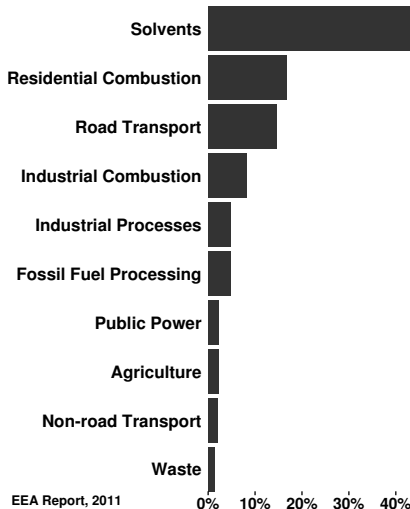
Comparison of  $O_3$  Production in Chemical Mechanisms

**Impact of Solvent Speciations on  $O_3$**

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# Motivation





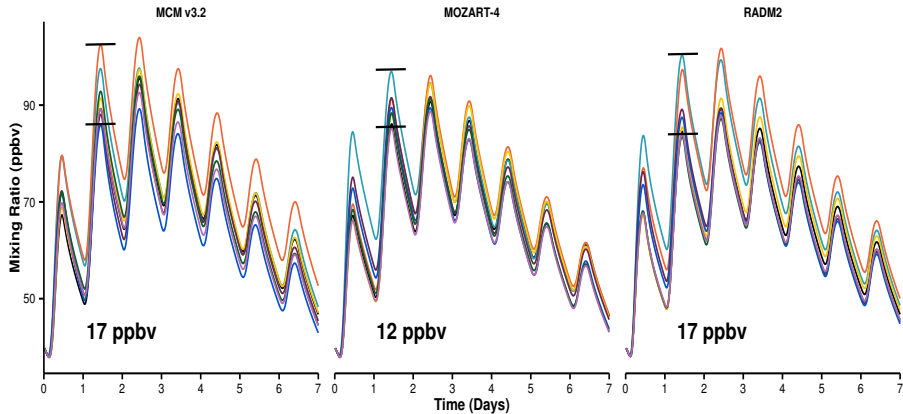
# Compared Solvent Speciations

Speciation	Reference
TNO	[Builtjes et al., TNO Report, 2002]
IPCC	[Ehhalt et al., IPCC Report, 2001]
EMEP	[Simpson et al., ACP, 2010]
DE94	[Friedrich et. al., JAC, 2002]
GR95	[Sidiropoulos and Tsilingiridis, FEB, 2007]
GR05	[Sidiropoulos and Tsilingiridis, FEB, 2007]
UK98	[Goodwin, UK NAEI report, 2000]
UK08	[Murrells et al., UK NAEI Report, 2010]

- ▶ MECCA boxmodel over 7 days.
- ▶ Idealised urban area of 1000 km<sup>2</sup>.
- ▶ Solvent sector contributes 43 % to total NMVOC emissions (1000 tons/day) [Warnecke et al., JGR, 2007].  
Total NMVOC emissions of 430 tons/day.
- ▶ NMVOC emissions constant until noon of day 1.
- ▶ NO source tuned for maximum ozone production.

## Ozone Mixing Ratio Time Series

— TNO — IPCC — EMEP — DE94 — GR95 — GR05 — UK98 — UK08

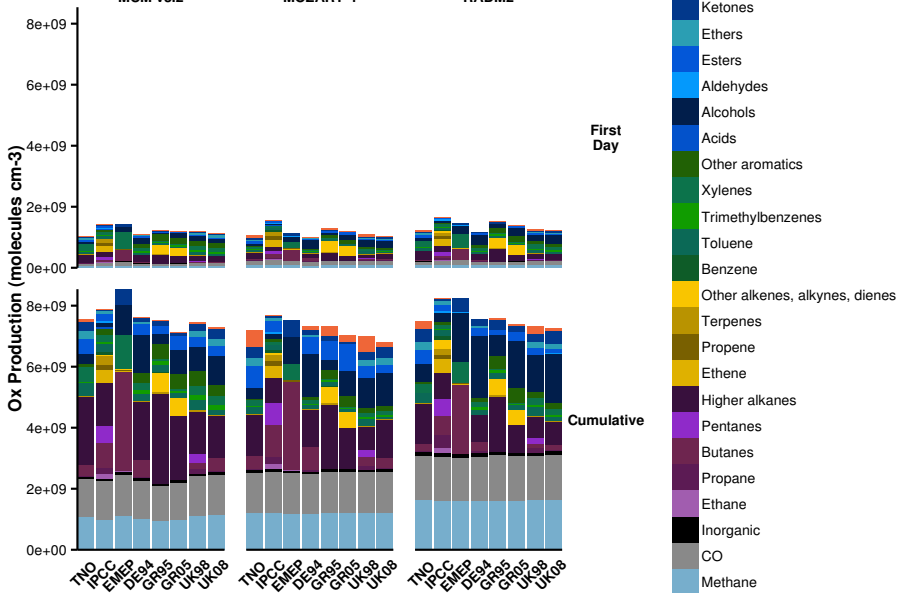


# First Day and Cumulative Allocated Ox Production

MCM v3.2

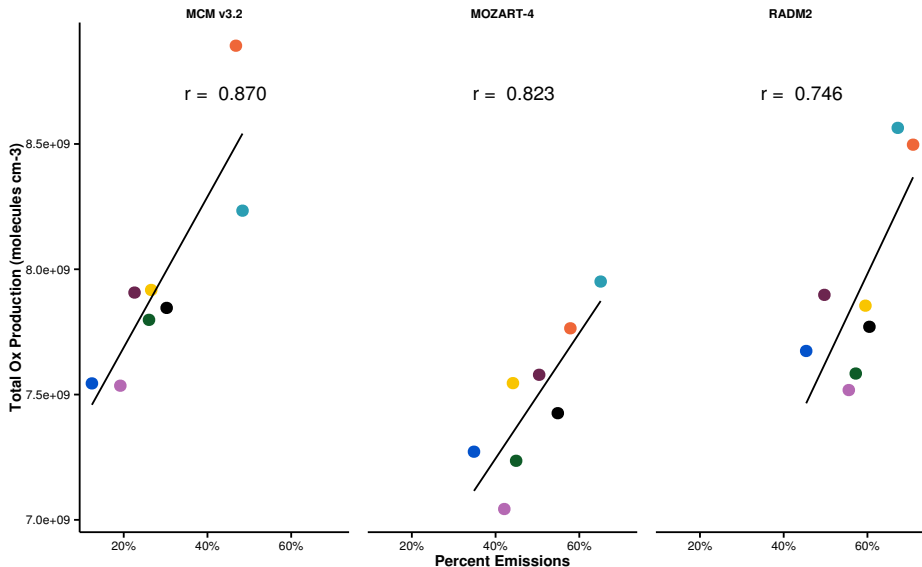
MOZART-4

RADM2



# Correlation of Cumulative Ox Production and Alkane Emissions

● TNO ● IPCC ● EMEP ● DE94 ● GR95 ● GR05 ● UK98 ● UK08



- ▶ Prepared an initial draft focussing on modelling work.
- ▶ Erika will be first author.
- ▶ Final paper will include more background information on comparing the different solvent sector speciations.
- ▶ Submit to Atmospheric Environment by end-August.

Previous Meeting Re-cap

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Impact of Solvent Speciations on  $O_3$

**Sensitivity of  $O_3$  Production on Modelled Conditions**

Timeline

- ▶ MECCA boxmodel over 7 days.
- ▶ Initial NMVOC typical of Los Angeles.
- ▶ NO source tuned for maximum  $O_3$  production.



- ▶ Tagging follows organic products from VOC degradation  
⇒ effects on  $O_3$  production inferred from  $O_x$  production.
- ▶ Constant PBL height of 1 km  
⇒ no dilution or vertical mixing.
- ▶ Constant temperature of 293 K.

# 1. Tagging Approach

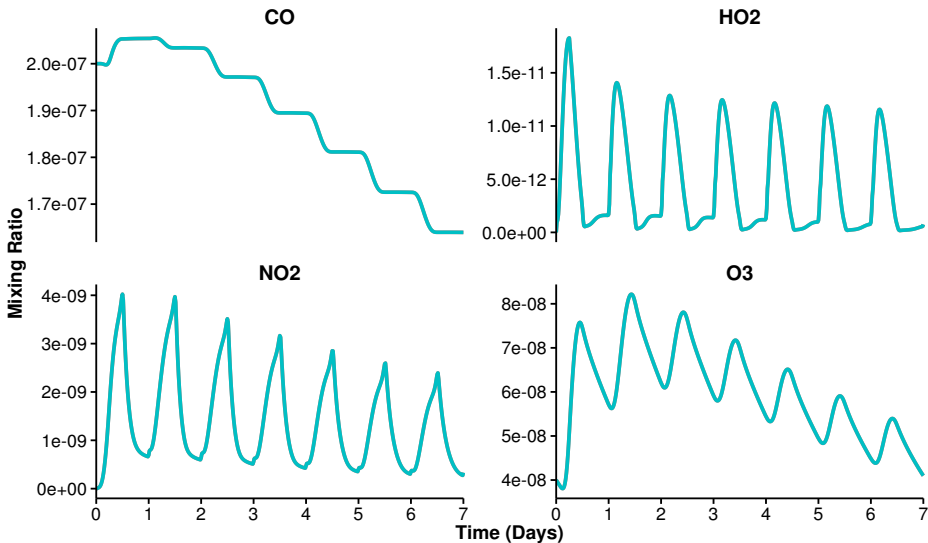
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- ▶ VOC tagging approach implemented in global model by Shuai and Tim.
- ▶ Allows allocation of  $O_3$  mixing ratios to source rather than comparing  $O_x$  production.
- ▶ Tagged MOZART-4 mechanism that was implemented in boxmodel for mechanism comparison study.

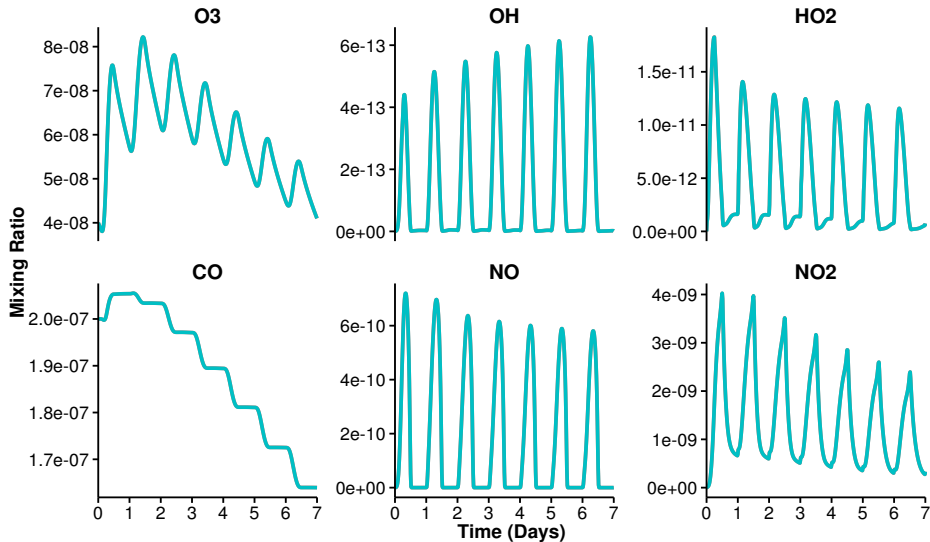
## Real vs Tagged Mixing Ratios

— Non-tagged — Tagged



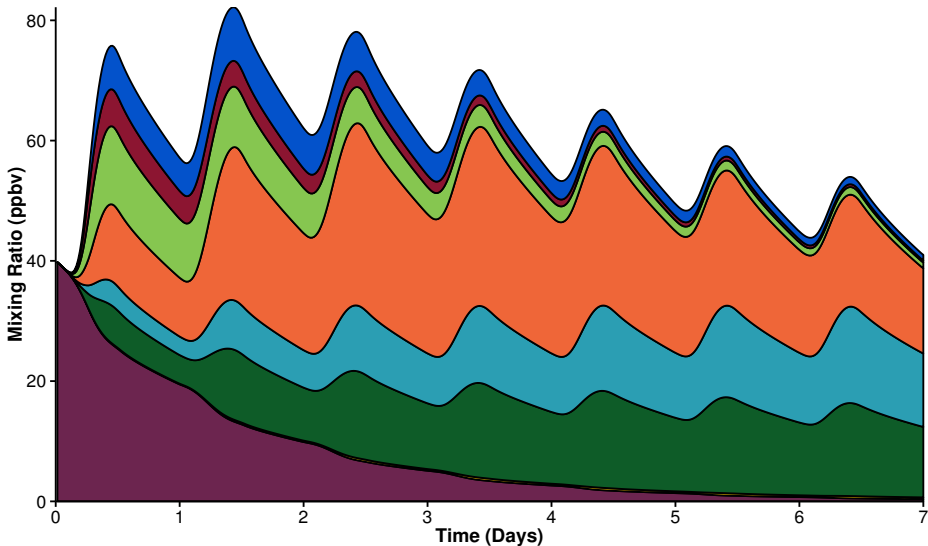
## Mixing Ratio Comparison between Old and New Tagging

new\_tagging old\_tagging



## Source Allocation of Ozone Mixing Ratios

Aromatics Isoprene Alkenes Alkanes CH<sub>4</sub> CO XTR INI



## 2. Low and High NO<sub>x</sub> Conditions

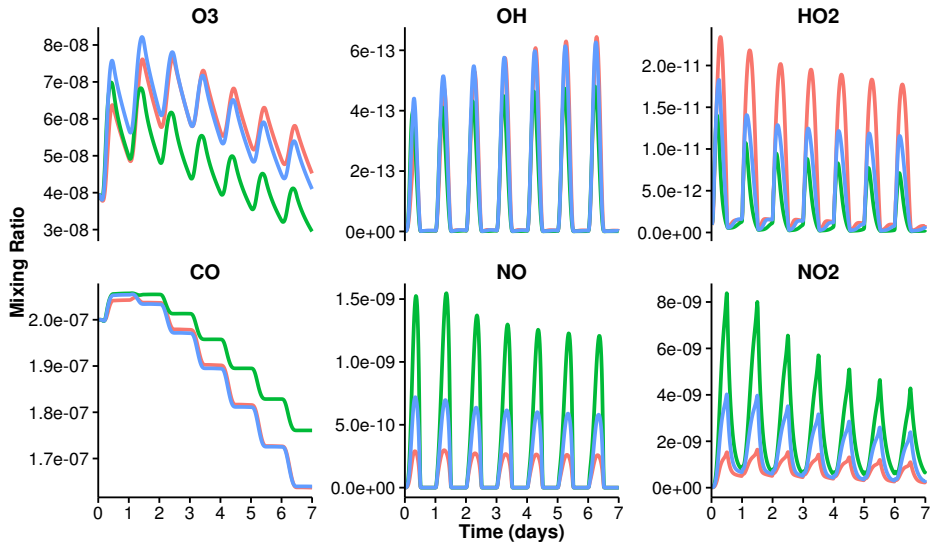
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- ▶ Modelling rural and polluted urban conditions.
- ▶ MOZART-4 mechanism with VOC tagging approach.
- ▶ NO emissions calculated for maximum O<sub>3</sub> production scaled
  - ▶ 0.5 for Low NO<sub>x</sub>
  - ▶ 1.5 for High NO<sub>x</sub>

# Mixing Ratio Comparisons in Different Atmospheric Regimes

— NOx\_limited — NOx\_saturated — Tuned



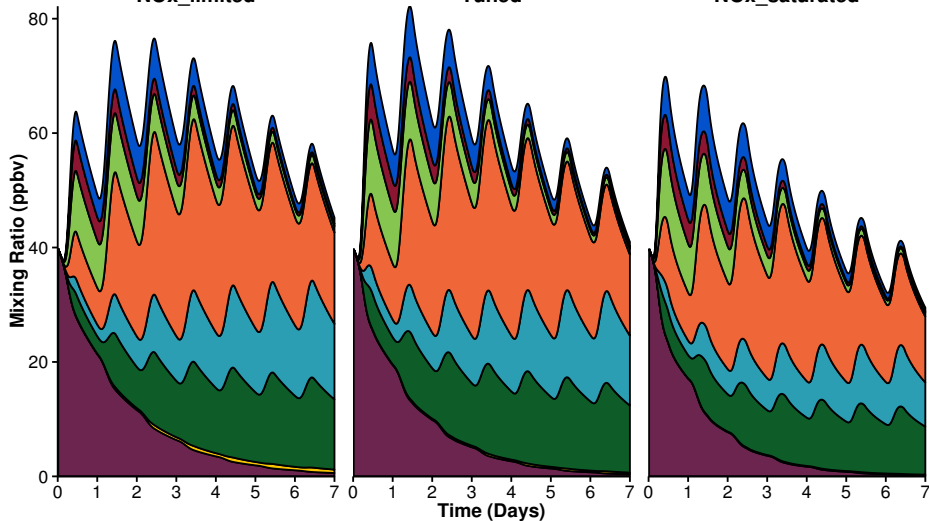
## Allocated Ozone Mixing Ratios

Aromatics Isoprene Alkenes Alkanes CH<sub>4</sub> CO XTR INI

NO<sub>x</sub>\_limited

Tuned

NO<sub>x</sub>\_saturated

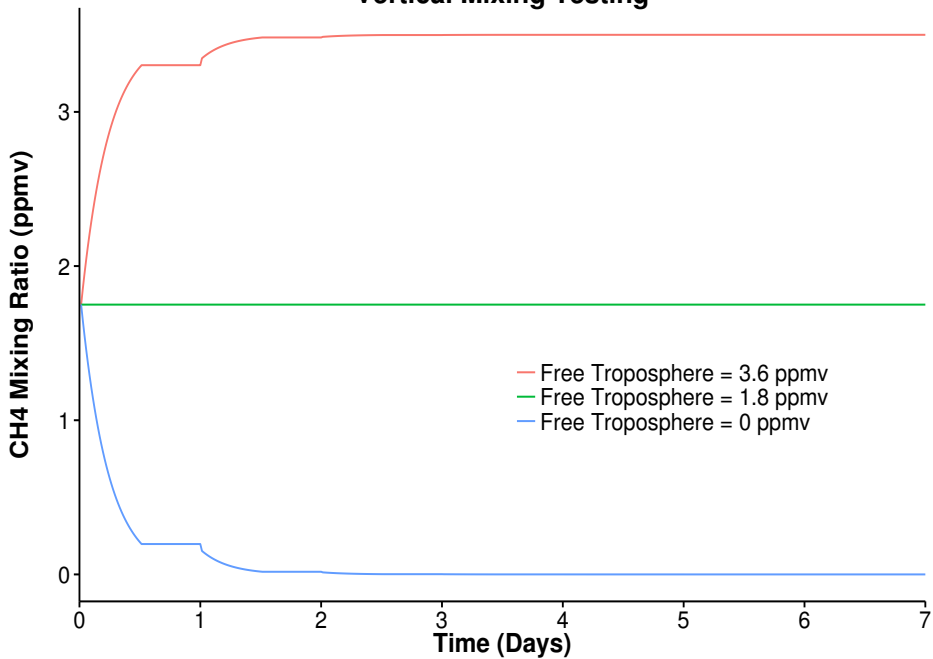




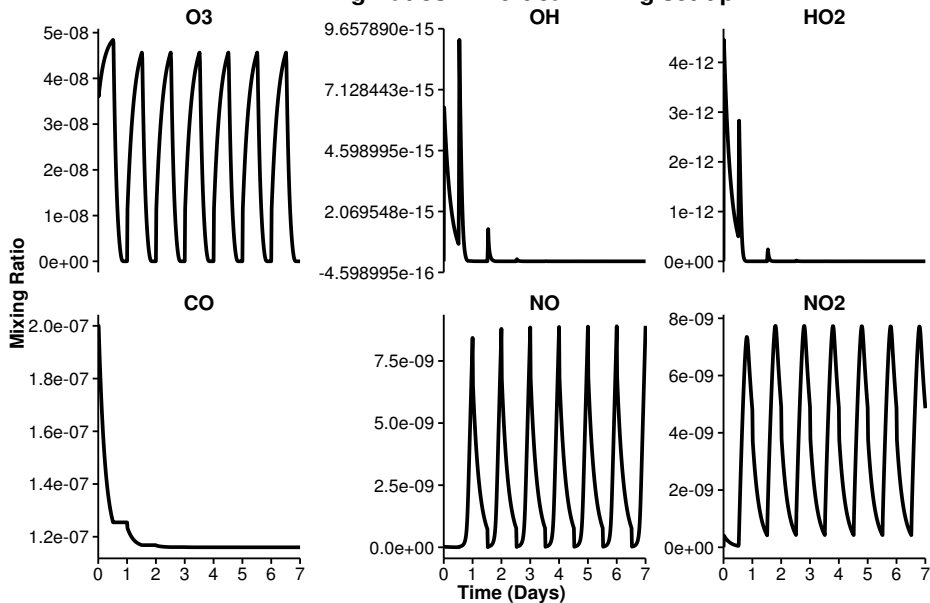
### 3. Vertical Mixing

- ▶ Included diurnal cycle for PBL height from CARES measurement campaign.
- ▶ Vertical mixing with free troposphere approach from Sandra Louren's thesis.
- ▶ Free troposphere mixing ratios for  $O_3$  and CO from MATCH-MPIC model.

## Vertical Mixing Testing



## Mixing Ratios in Vertical Mixing set-up



## 4. Temperature

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- ▶ Run boxmodel at 295 K, scenario of a warmer climate.
- ▶ Compare  $O_3$  between lower and higher temperatures.
- ▶ According to recent review by Pusede et al., temperature dependent chemistry of alkyl nitrates impacts  $O_3$  production.
- ▶ Assess how this chemistry is represented in the chemical mechanisms used in comparison study.

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**Timeline**

- ▶ Submit solvents sector emissions paper by end-August 2015.
- ▶ Finish sensitivity study paper by end-Dec 2015.
- ▶ Present sensitivity study at AGU in December 2015.
- ▶ Hand in thesis to reviewers by end-April 2016.
- ▶ Six weeks for reviewers to assess thesis.
- ▶ Display graded thesis at FU Examinations Office for 2 weeks prior to thesis defense.
- ▶ Defend thesis in July 2016.