Launch of AQEG report: Ozone in the United Kingdom, 3rd March 2009

Simulating concentrations of isoprene and other hydrocarbons in TORCH 2003 using a Photochemical Trajectory Model

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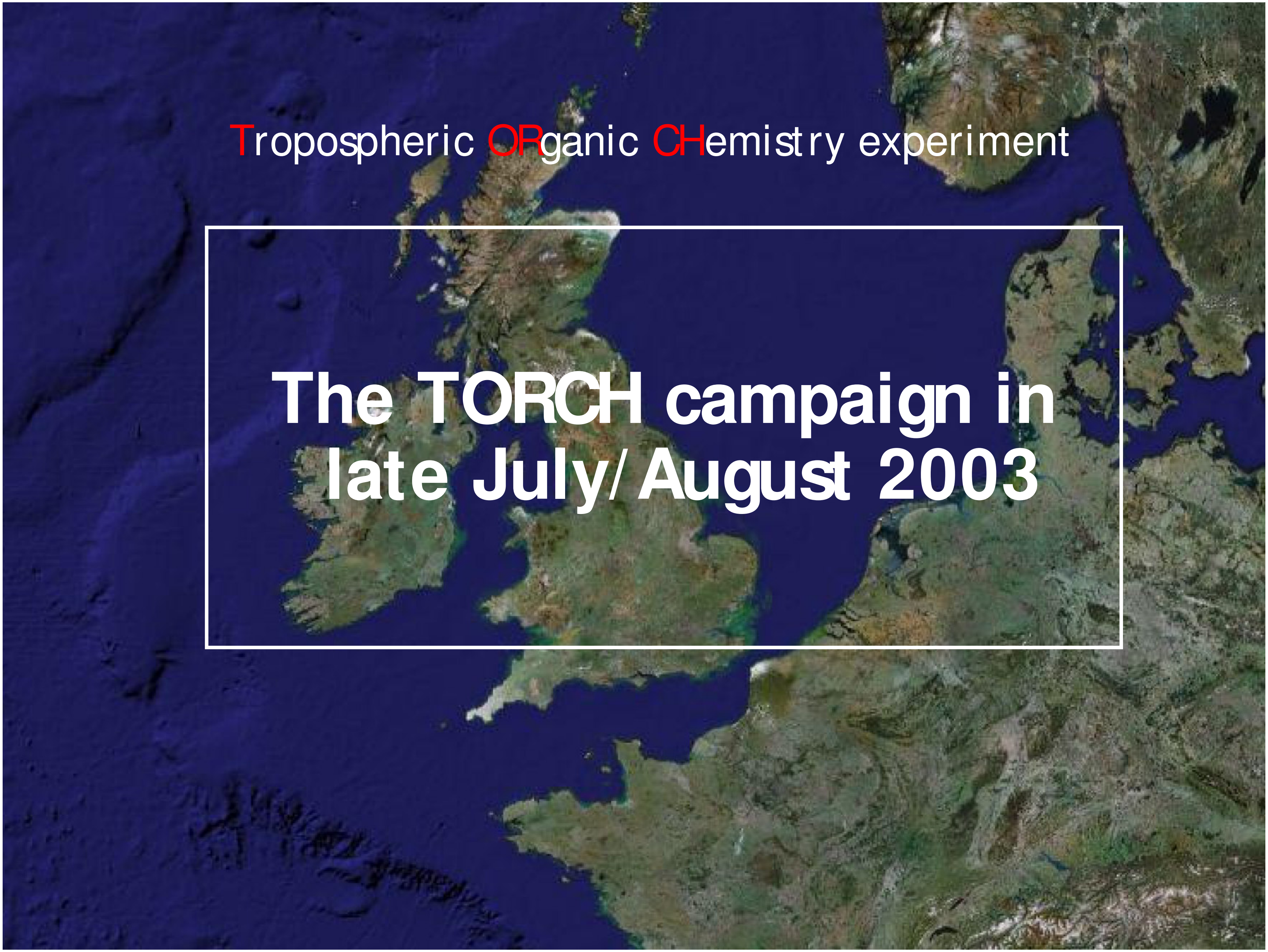
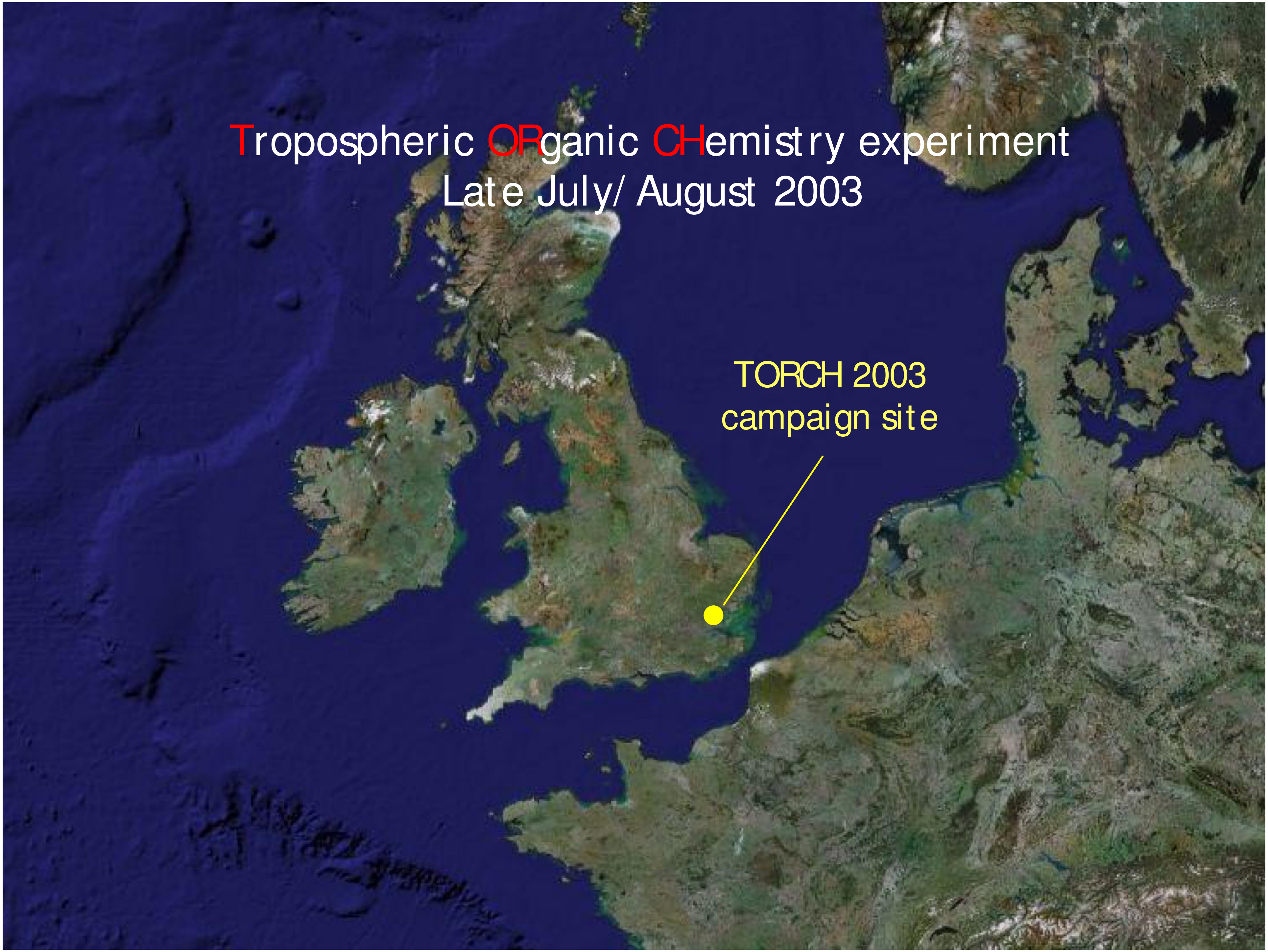
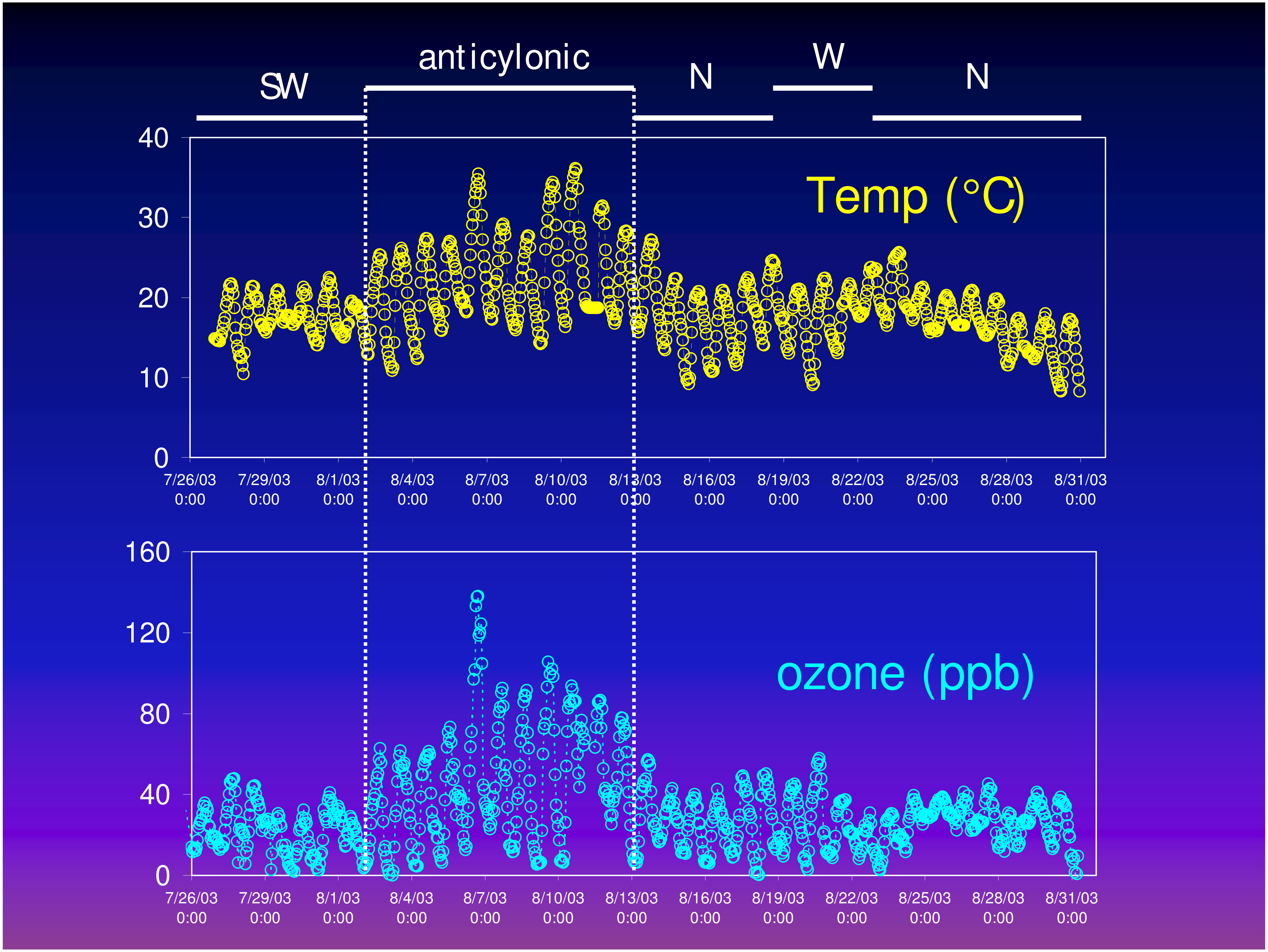
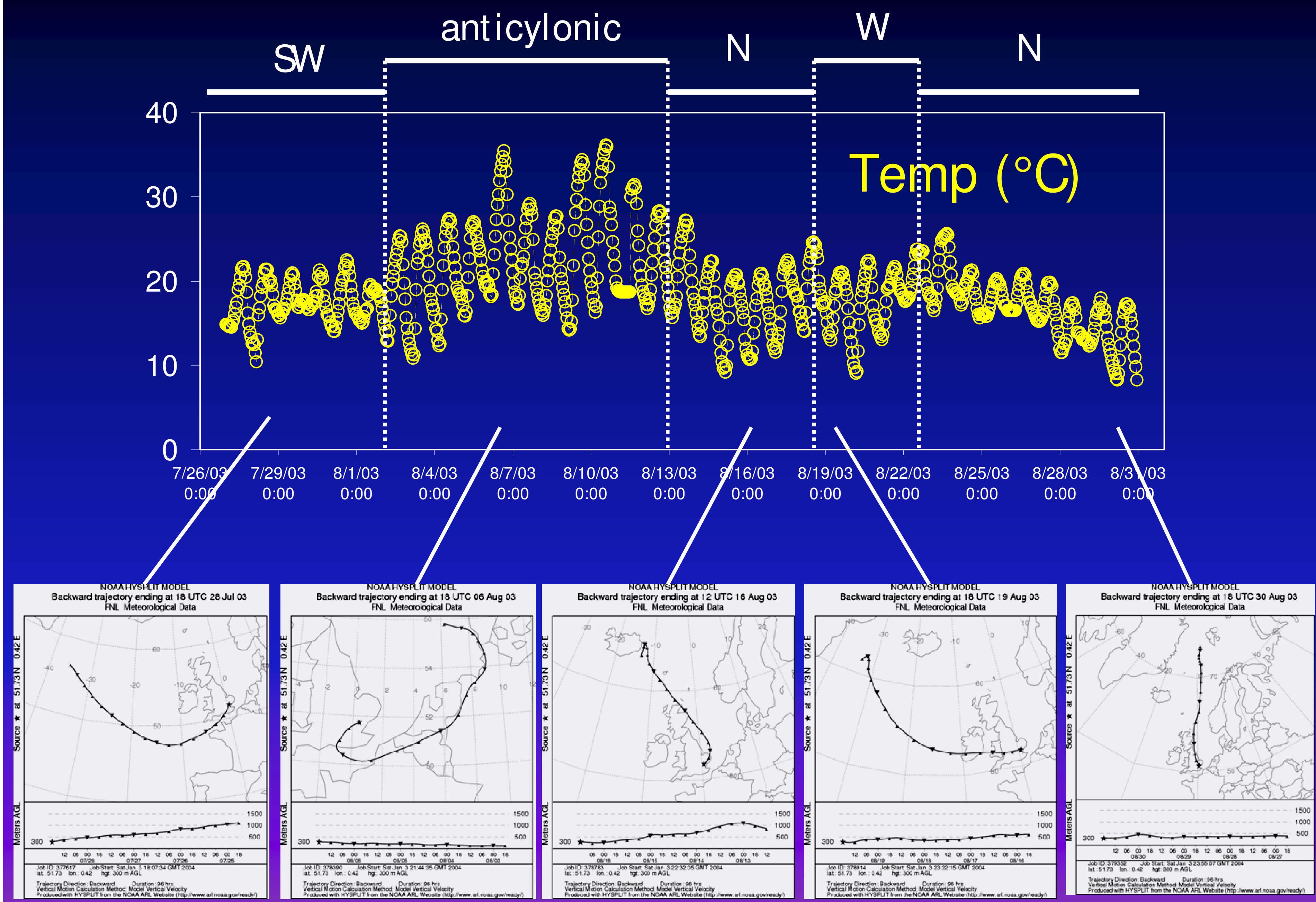
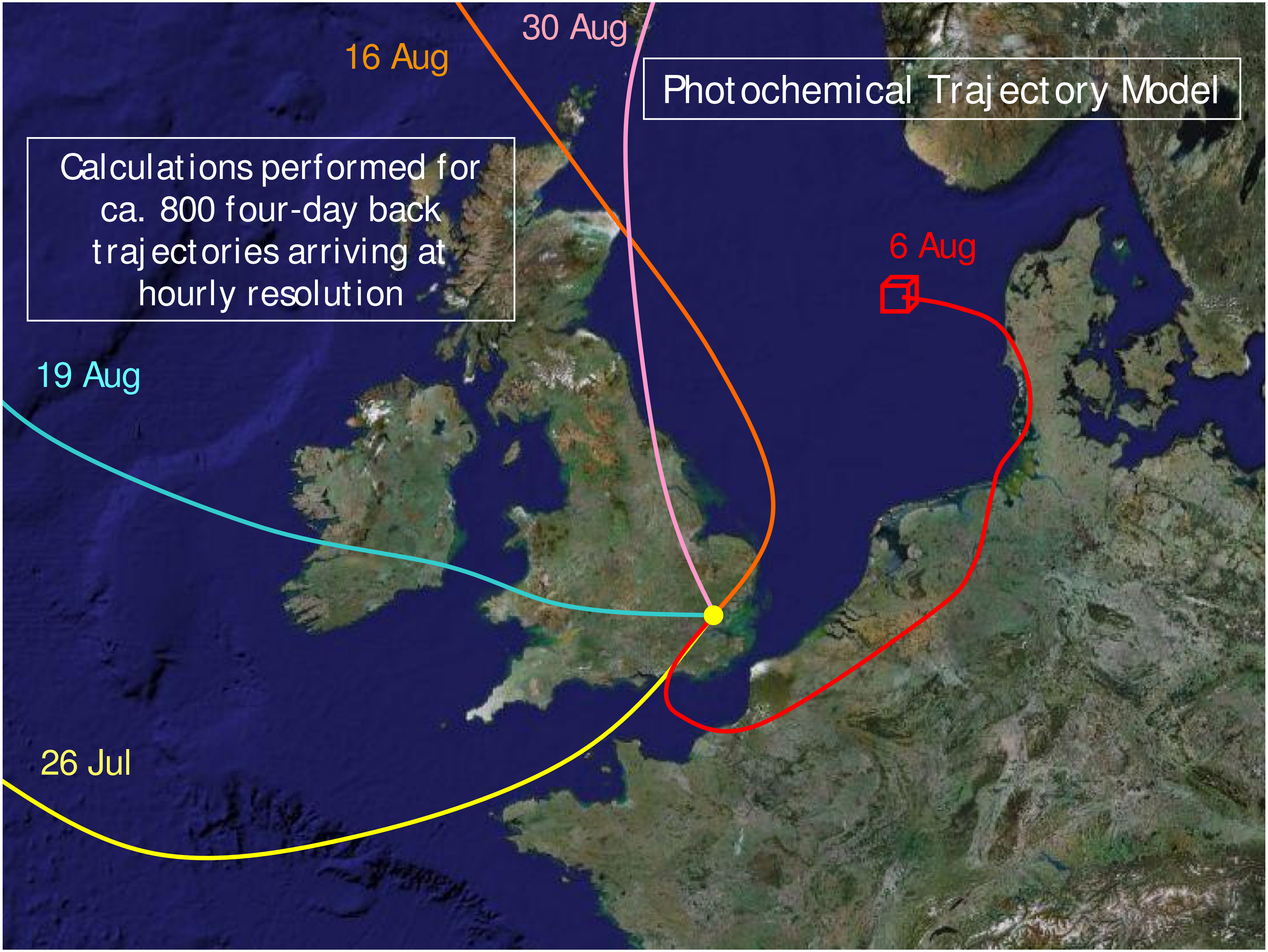

Tropospheric ORganic CHemistry experiment
The TORCH campaign in late July/August 2003


TRopospheric ORganic CHemistry experiment
Late July/ August 2003
TORCH 2003
campaign site


SW
anticylonic
N
W
N
Temp (°C)
40
30
20
10
0
7/26/03 0:00
7/29/03 0:00
8/1/03 0:00
8/4/03 0:00
8/7/03 0:00
8/10/03 0:00
8/13/03 0:00
8/16/03 0:00
8/19/03 0:00
8/22/03 0:00
8/25/03 0:00
8/28/03 0:00
8/31/03 0:00
ozone (ppb)
160
120
80
40
0



Example trajectories


Photochemical Trajectory Model
Calculations performed for ca. 800 four-day back trajectories arriving at hourly resolution
30 Aug
16 Aug
6 Aug
19 Aug
26 Jul

Emissions | Photochemical Trajectory Model

Emissions of NO_X, speciated VOCs, CH_4, CO and SO_2

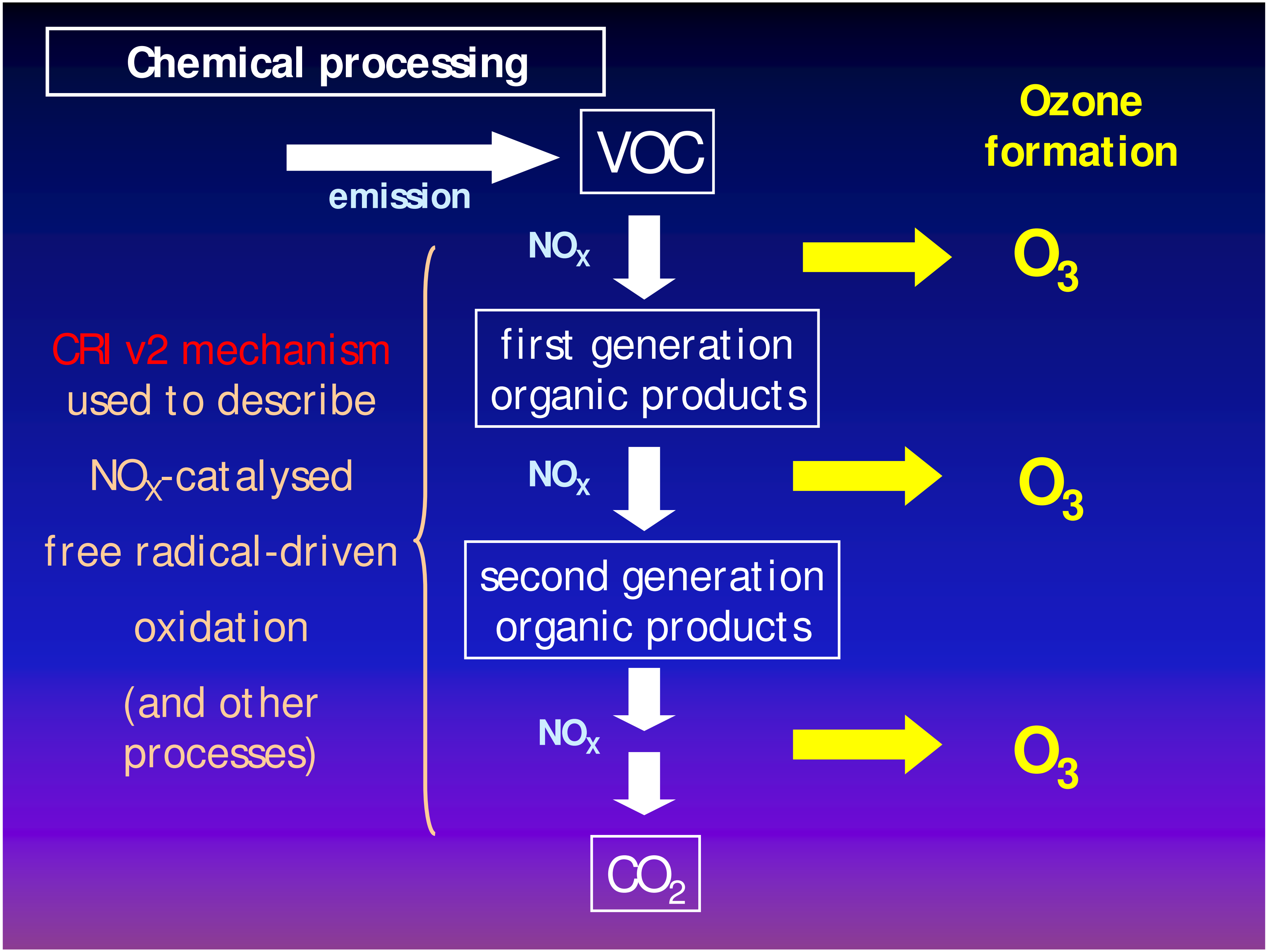
Anthropogenic:

- NAEI for UK, EMEP for outside UK.
- Seasonal, weekly and diurnal temporal factors applied.
- Detailed VOC speciation using 112 anthropogenic species.

Biogenic VOCs: Based on:

Dore, C., Hayman, G., Scholefield, P., Hewitt, N., Winiwarter, W. and Kressler, F. (2003). Mapping biogenic VOC emissions in England and Wales. Environment Agency R&D Technical Report E1-122/TR, ISBN 1-84432-092-8.

- Emissions potentials developed at 1 x 1km resolution for the whole of Europe. Aggregated to 50 x 50 km.
- Representation implemented into PTM by Garry Hayman (NPL)
- Full representation of temperature and PAR dependence
- VOC speciation represented by isoprene, α–pinene and β–pinene


Chemical processing
emission
VOC
Ozone formation
NOx
O3
CRI v2 mechanism used to describe NOx-catalysed free radical-driven oxidation (and other processes)
first generation organic products
NOx
O3
second generation organic products
NOx
O3
CO2

Chemical processing

The "*Common Representative Intermediates*" (CRI) mechanism
- Latest version: CRI v2

CRI v2

442 species

1191 reactions

Atmos. Environ., 42, 7185-7195, 2008

Degrades methane and 115 emitted VOCs

Chemical processing

The "*Common Representative Intermediates*" (CRI) mechanism
- Latest version: CRI v2

<u>CRI v2</u>

442 species

1191 reactions

Atmos. Environ., 42, 7185-7195, 2008

Degrades methane and 115 emitted VOCs

Traceable to..... the "*Master Chemical Mechanism*" (MCM)
- Latest version: MCM v3.1

<u>MCM v3.1</u>

5,900 species

13,500 reactions

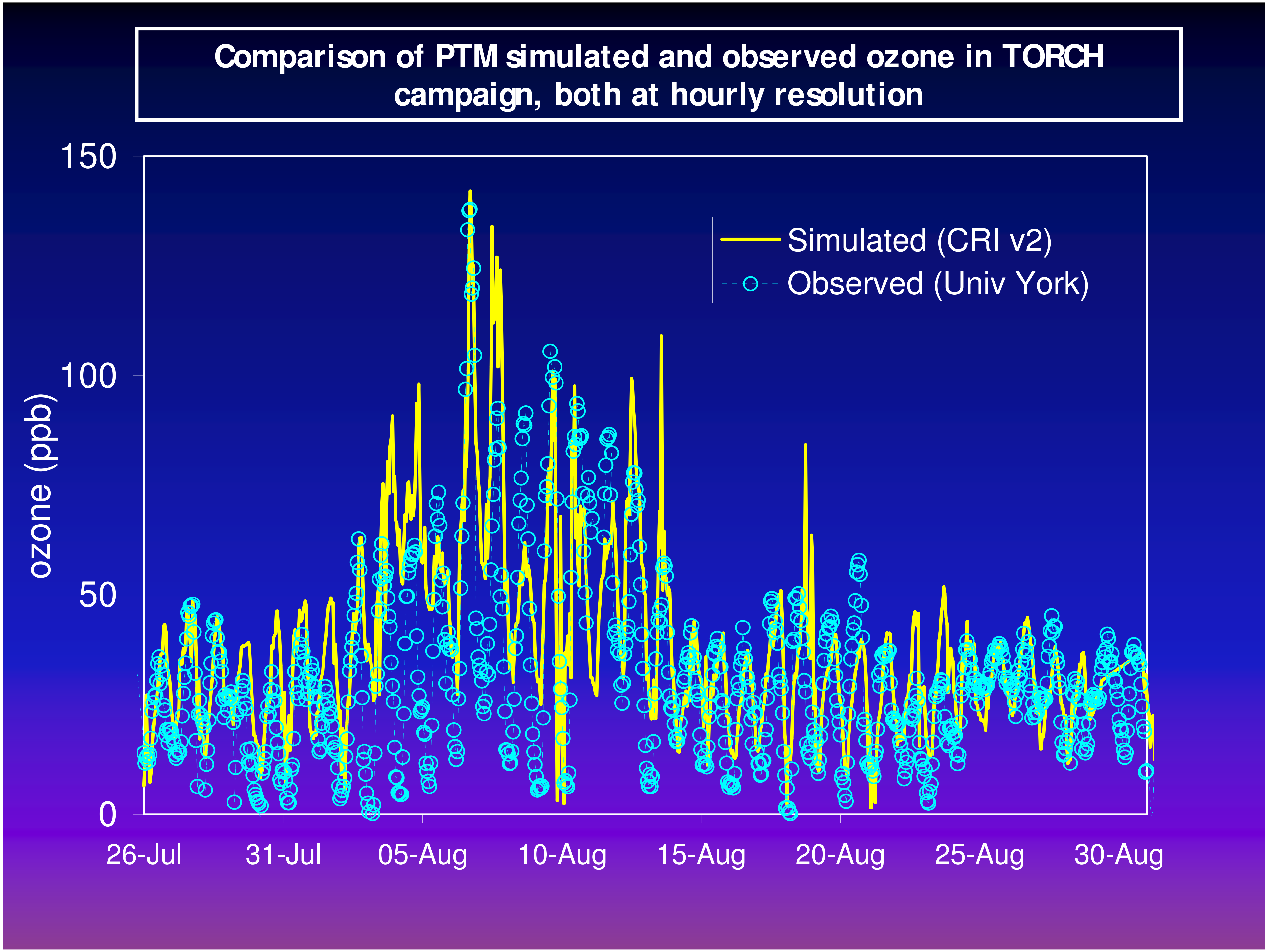
Atmos. Environ., **31**, 81-104, 1997

Atmos. Chem. Phys., **3**, 161-180, 2003

Atmos. Chem. Phys., **3**, 181-193, 2003

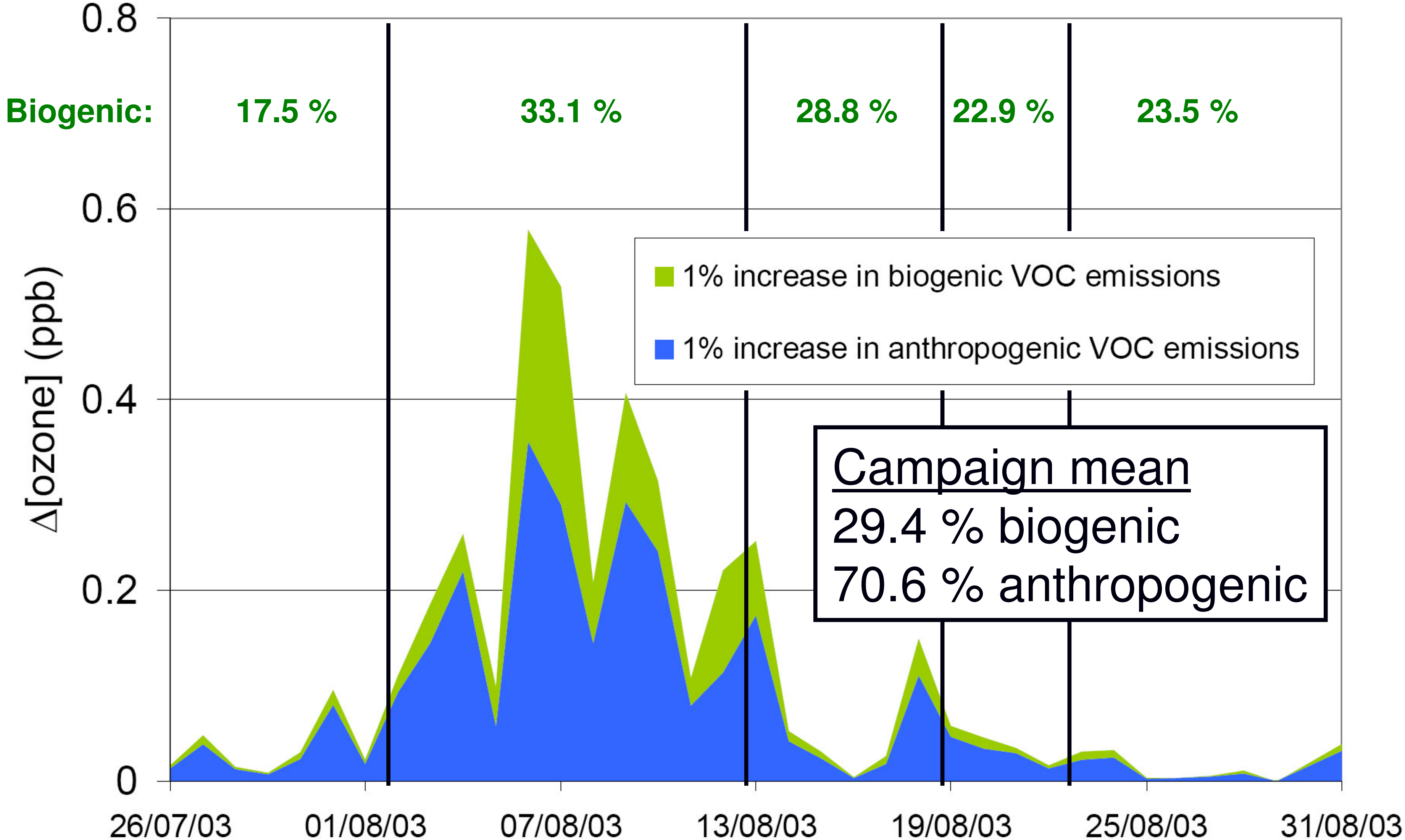
Atmos. Chem. Phys., 5, 641-664, 2005

Relative run time in PTM ≈ 320

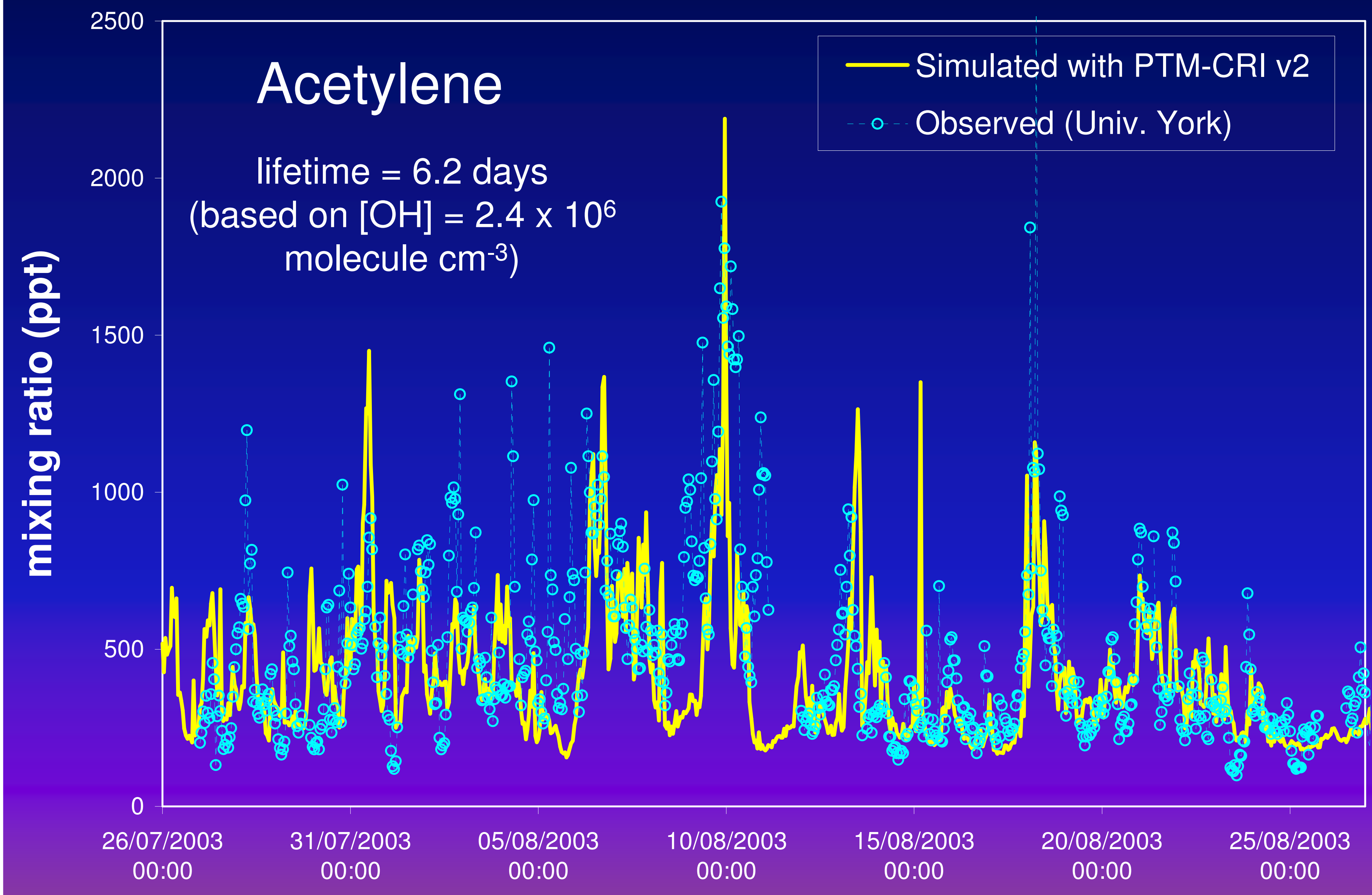


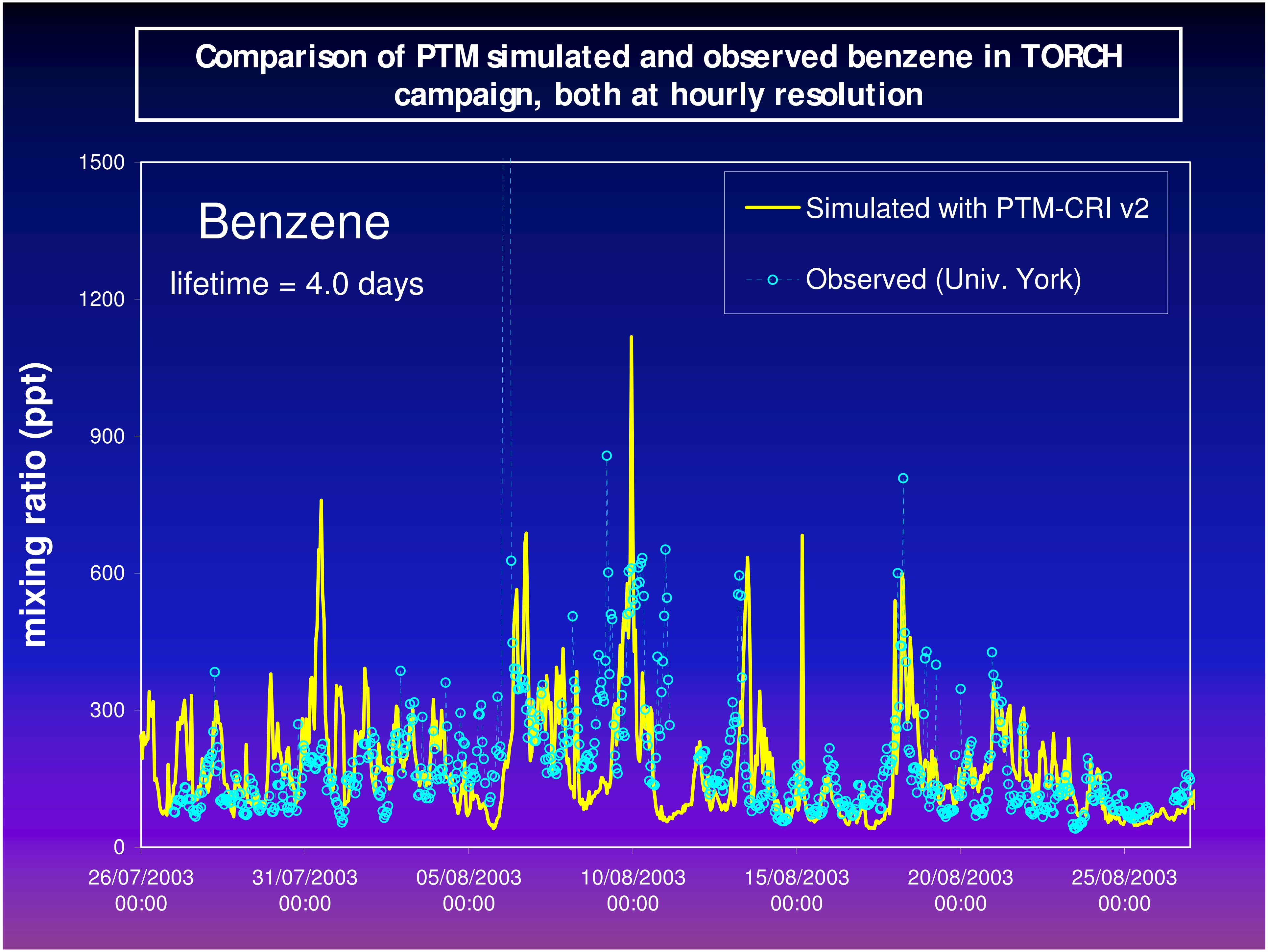
Comparison of PTM simulated and observed ozone in TORCH campaign, both at hourly resolution
Simulated (CRI v2)
Observed (Univ York)
ozone (ppb)
150
100
50
0
26-Jul
31-Jul
05-Aug
10-Aug
15-Aug
20-Aug
25-Aug
30-Aug

Relative contributions of regional-scale biogenic and anthropogenic VOC emissions to ozone formation



Comparison of PTM simulated and observed acetylene in TORCH campaign, both at hourly resolution

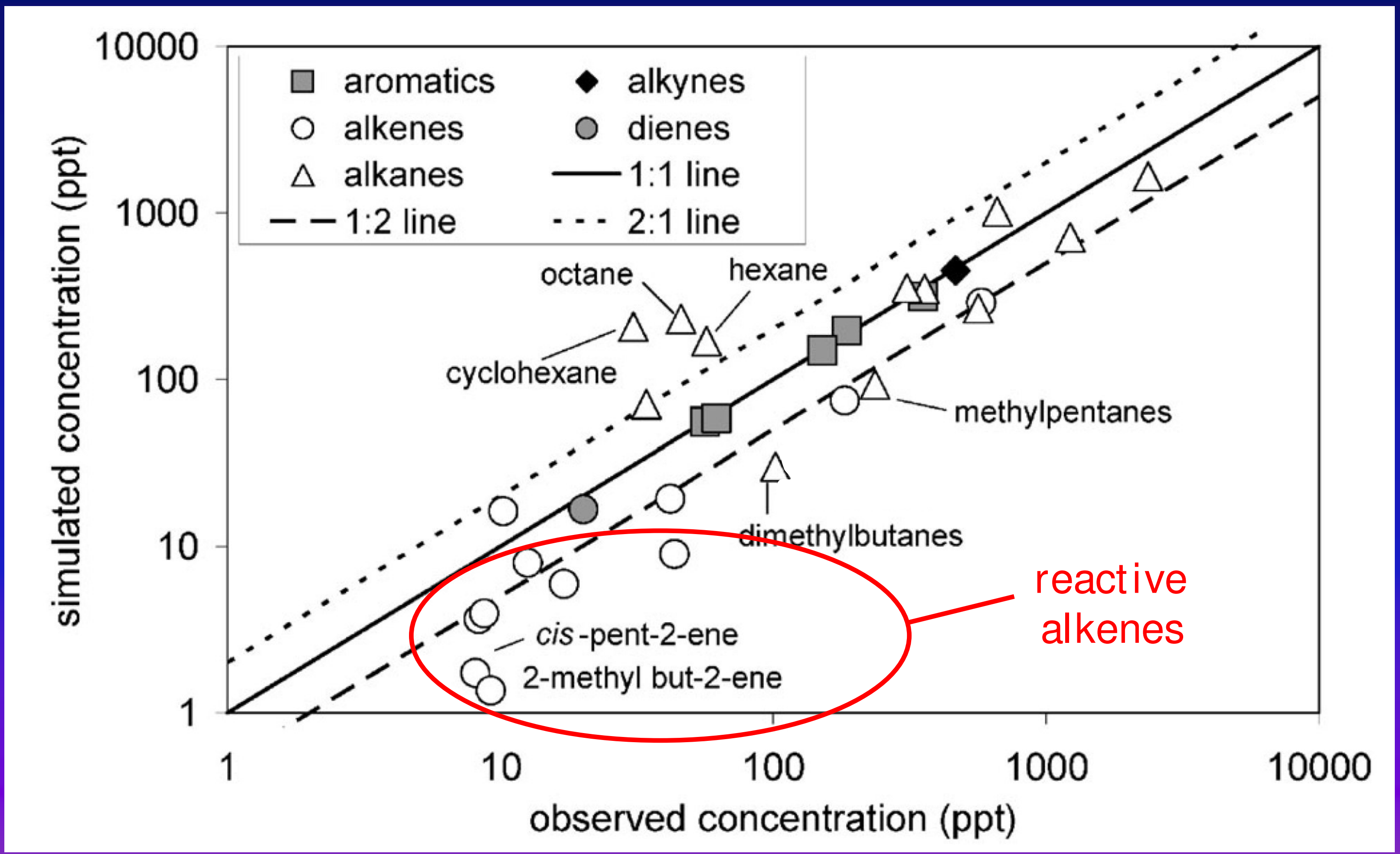


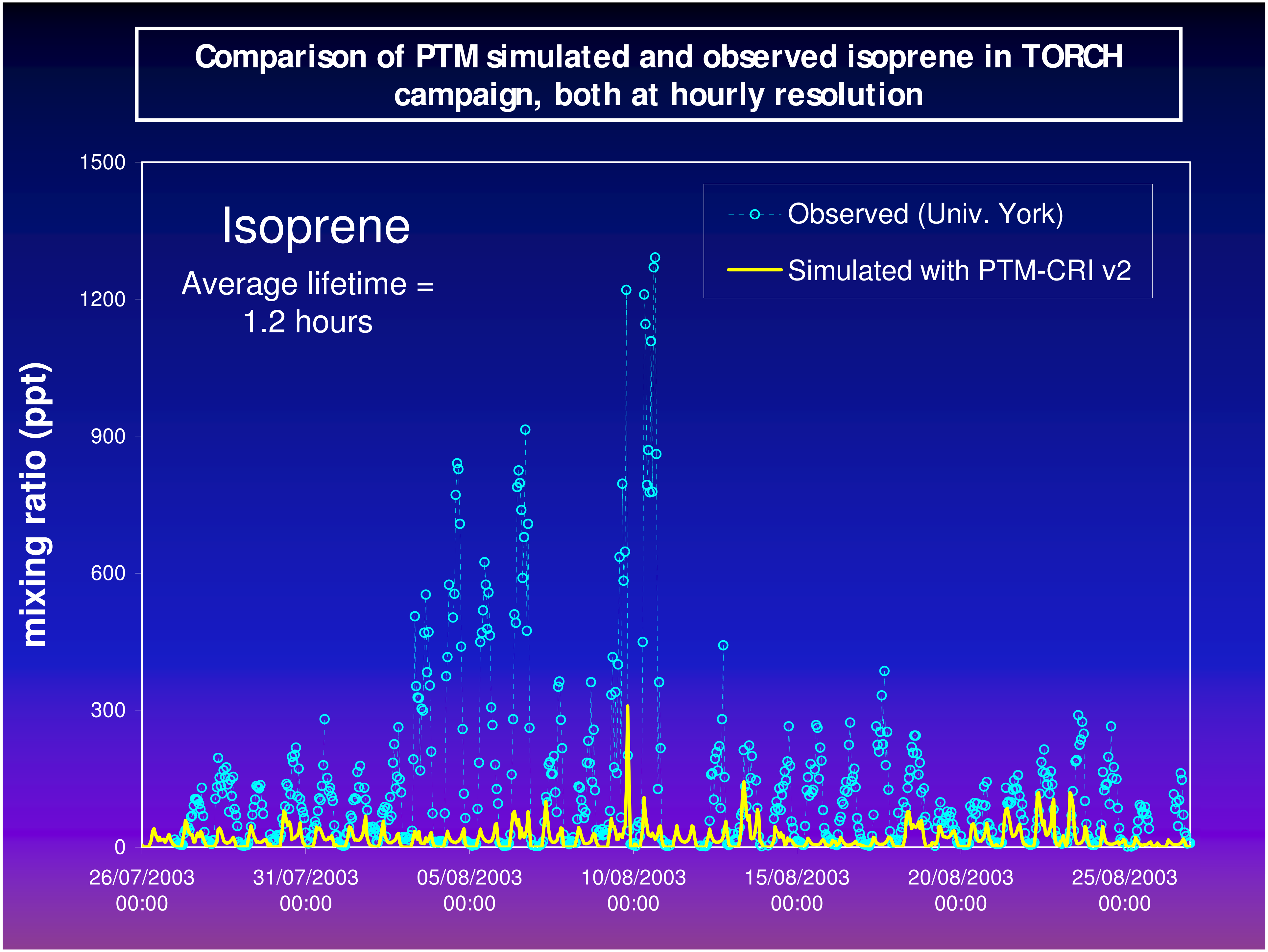


Comparison of PTM simulated and observed benzene in TORCH campaign, both at hourly resolution
Benzene
lifetime = 4.0 days
Simulated with PTM-CRI v2
Observed (Univ. York)
mixing ratio (ppt)
1500
1200
900
600
300
0
26/07/2003 00:00
31/07/2003 00:00
05/08/2003 00:00
10/08/2003 00:00
15/08/2003 00:00
20/08/2003 00:00
25/08/2003 00:00

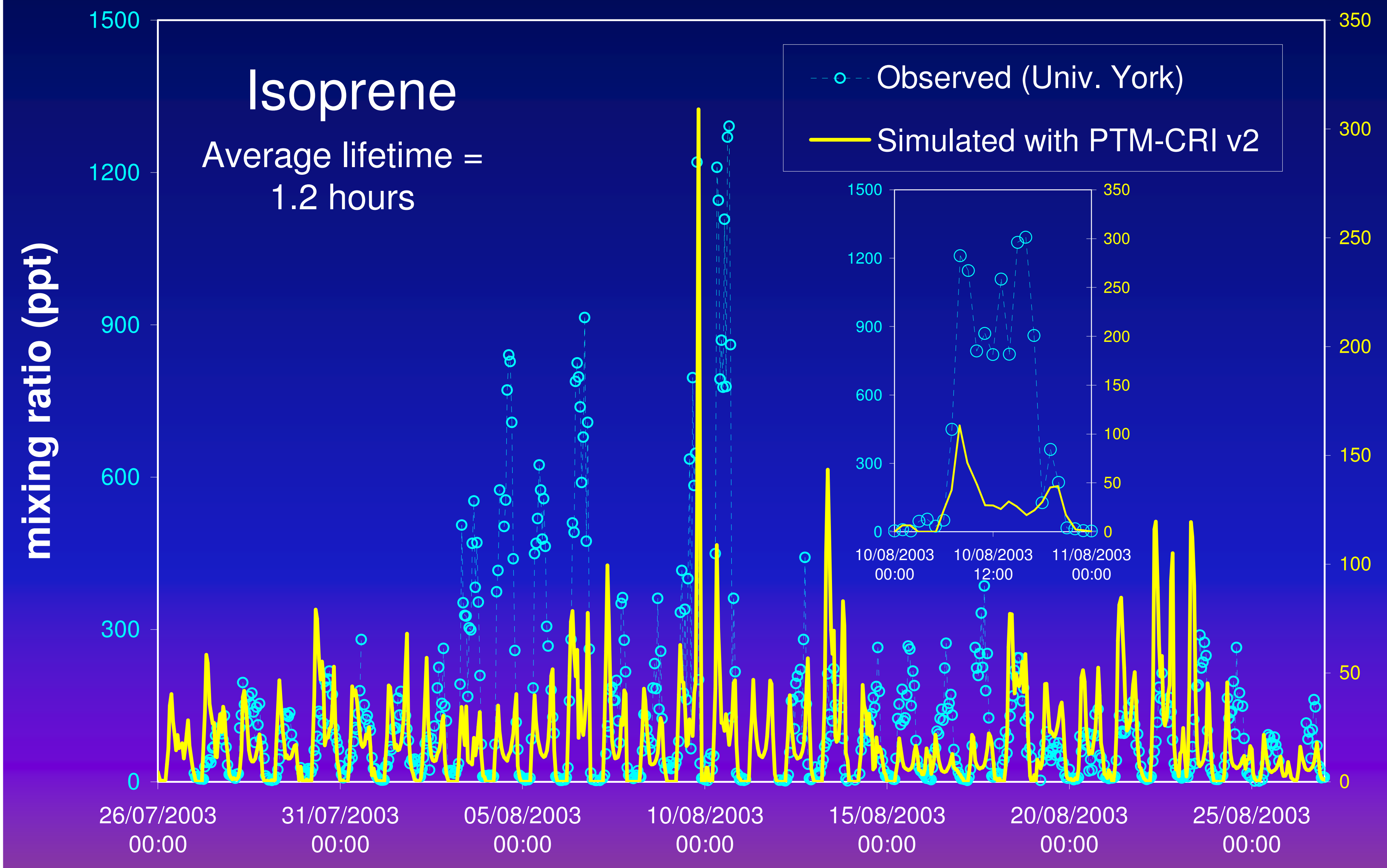
Campaign mean concentrations of 33 emitted anthropogenic hydrocarbons observed (York) vs PTM simulated

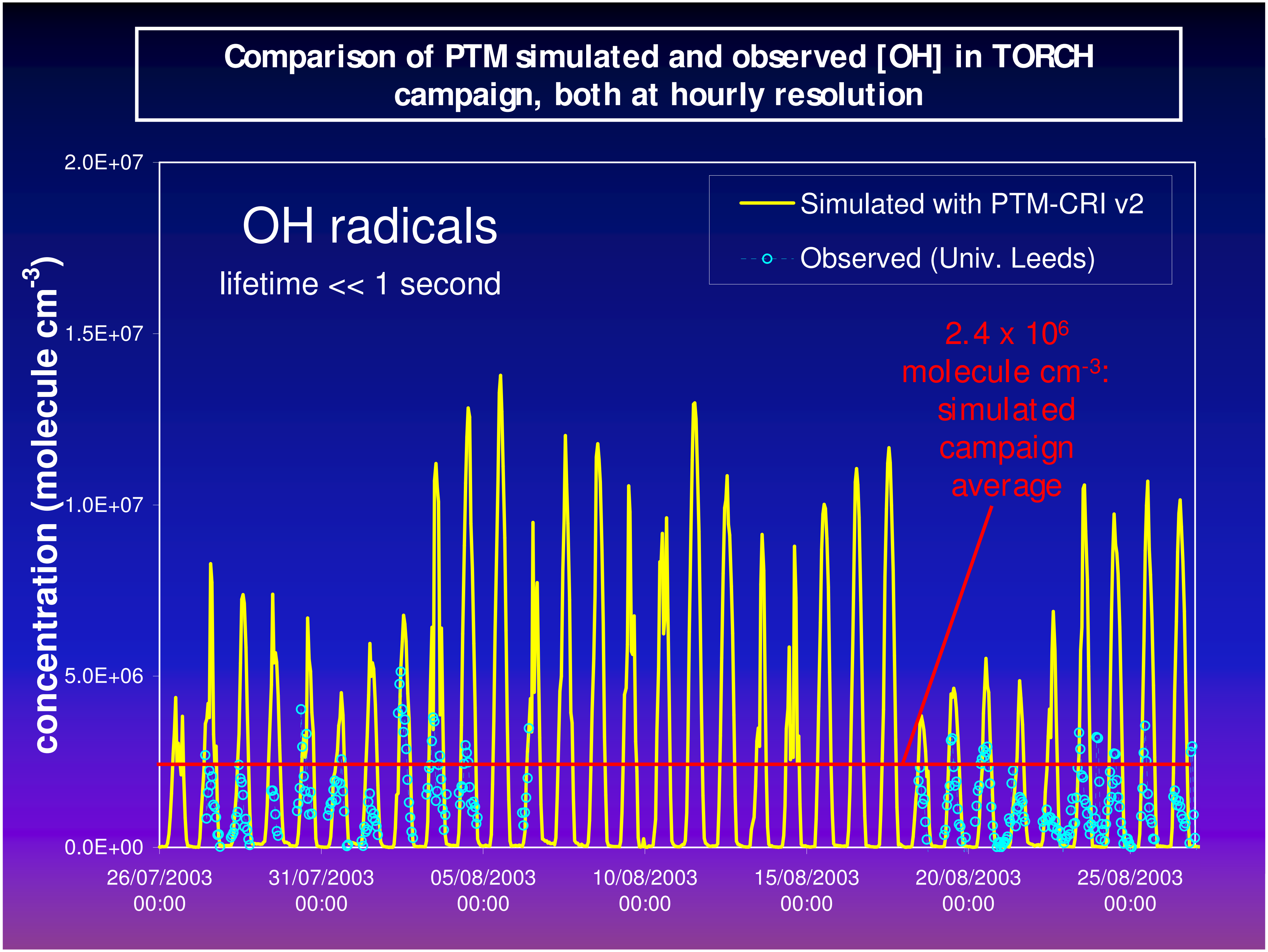
Taken from Utembe et al., Faraday Discussions, 130, 311-326, 2005



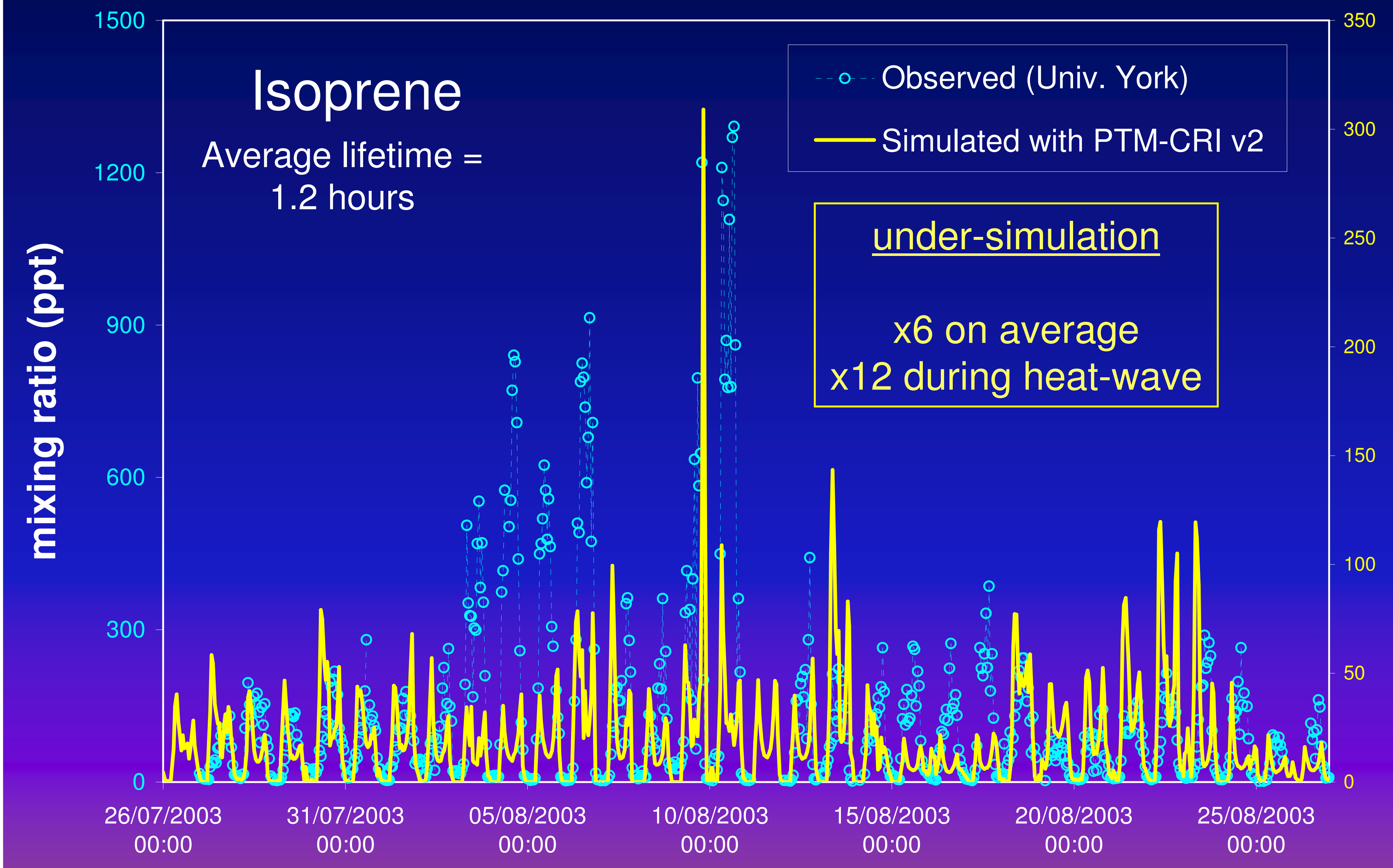

Comparison of PTM simulated and observed isoprene in TORCH campaign, both at hourly resolution
Isoprene
Average lifetime = 1.2 hours
Observed (Univ. York)
Simulated with PTM-CRI v2
mixing ratio (ppt)
1500
1200
900
600
300
0
26/07/2003 00:00
31/07/2003 00:00
05/08/2003 00:00
10/08/2003 00:00
15/08/2003 00:00
20/08/2003 00:00
25/08/2003 00:00

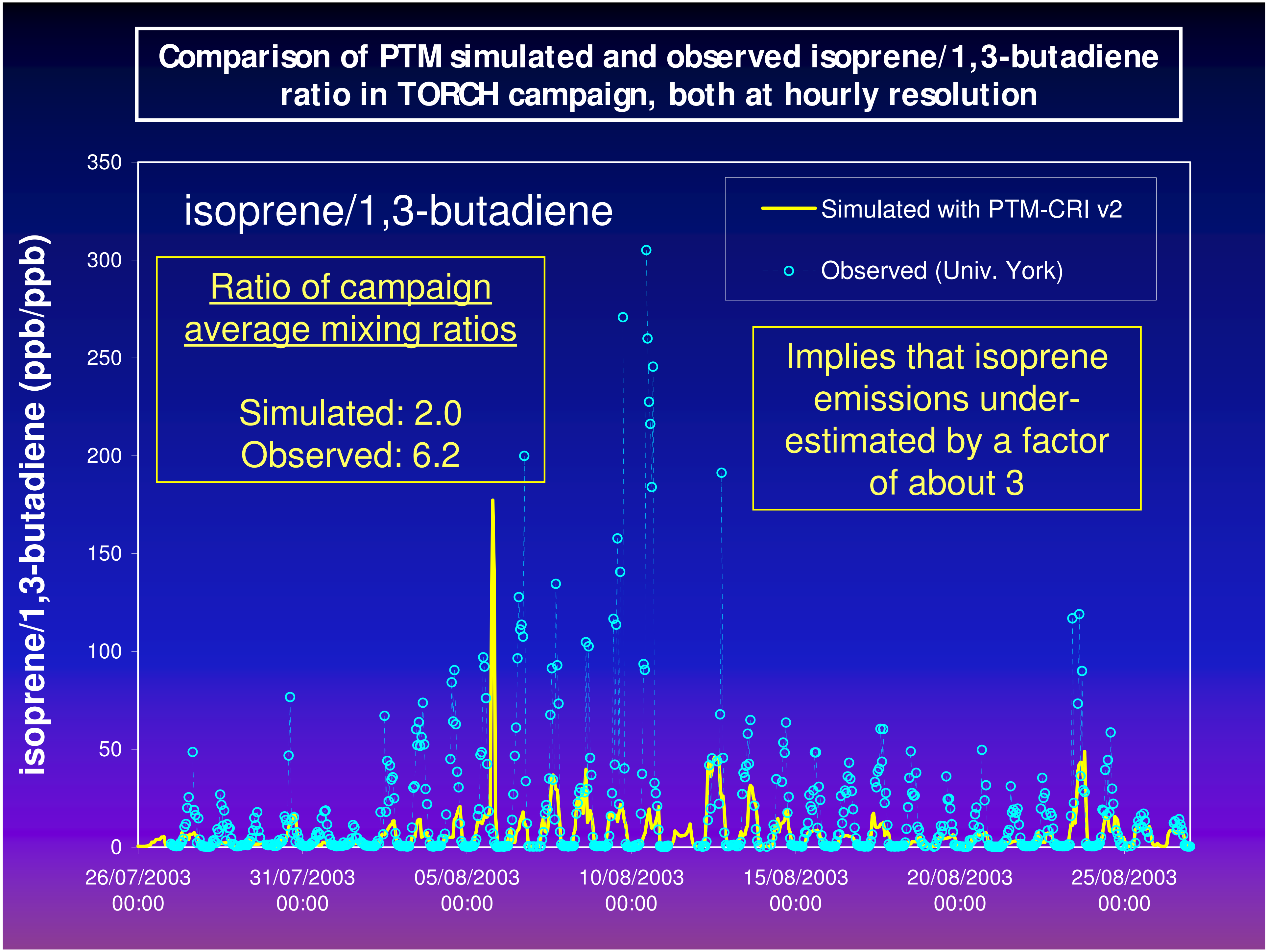
Comparison of PTM simulated and observed isoprene in TORCH campaign, both at hourly resolution




Comparison of PTM simulated and observed [OH] in TORCH campaign, both at hourly resolution
OH radicals
lifetime << 1 second
Simulated with PTM-CRI v2
Observed (Univ. Leeds)
2.4 x 10⁶ molecule cm⁻³: simulated campaign average
concentration (molecule cm⁻³)
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
26/07/2003 00:00
31/07/2003 00:00
05/08/2003 00:00
10/08/2003 00:00
15/08/2003 00:00
20/08/2003 00:00
25/08/2003 00:00

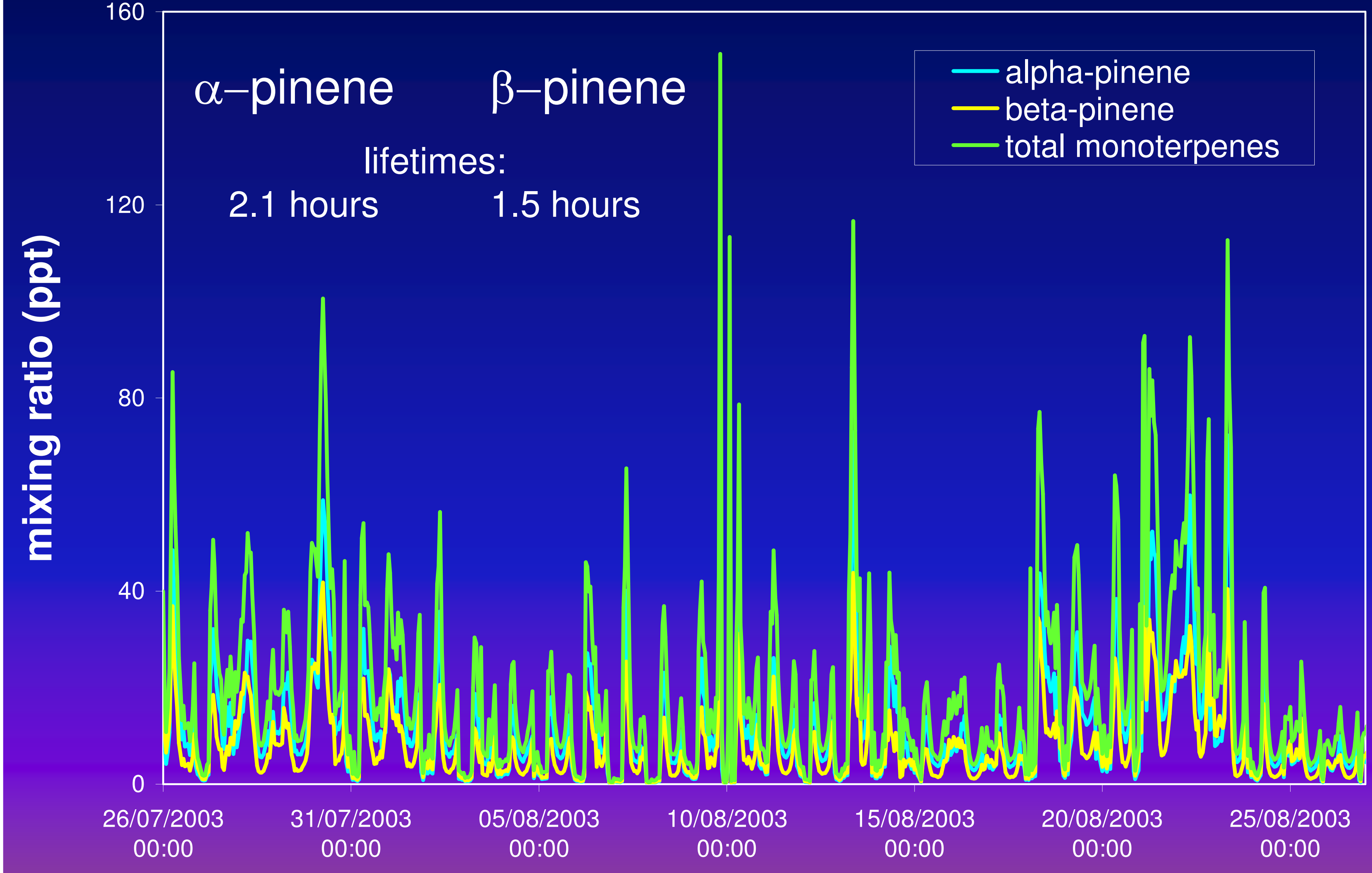
Comparison of PTM simulated and observed isoprene in TORCH campaign, both at hourly resolution





Comparison of PTM simulated and observed isoprene/1,3-butadiene ratio in TORCH campaign, both at hourly resolution
isoprene/1,3-butadiene
Ratio of campaign average mixing ratios
Simulated: 2.0
Observed: 6.2
Simulated with PTM-CRI v2
Observed (Univ. York)
Implies that isoprene emissions under-estimated by a factor of about 3
isoprene/1,3-butadiene (ppb/ppb)
350
300
250
200
150
100
50
0
26/07/2003 00:00
31/07/2003 00:00
05/08/2003 00:00
10/08/2003 00:00
15/08/2003 00:00
20/08/2003 00:00
25/08/2003 00:00

PTM simulation of other biogenics: representative monoterpenes, α– and β–pinene



Summarising remarks

- Trajectory model simulations of the TORCH-2003 campaign using a detailed VOC speciation and comprehensive chemistry yields reasonably good agreement between simulated and observed levels of a number of less reactive emitted anthropogenic hydrocarbons.
- Some difficulties arise in simulating observed surface levels of reactive hydrocarbons, due to concentration gradients.
- For isoprene, strong vertical gradients undoubtedly contribute to the model-measurement discrepancy.
- Consideration of the isoprene/1,3-butadiene ratio suggests that the implemented representation of biogenic isoprene emissions probably underestimates the local source strength by a factor of about 3.
- Simulations suggest that other more complex hydrocarbons (i.e., monoterpenes), were likely present at a collective concentration comparable with that of isoprene.

Potential impact of forest fires in Portugal in summer 2003

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 113, D07307, doi:10.1029/2007JD009098, 2008

Click Here for Full Article

European surface ozone in the extreme summer 2003

S. Solberg,[1] Ø. Hov,[2] A. Søvde,[3] I. S. A. Isaksen,[3] P. Coddeville,[4] H. De Backer,[5] C. Forster,[6] Y. Orsolini,[1] and K. Uhse[7]

Received 26 June 2007; revised 24 September 2007; accepted 3 December 2007; published 10 April 2008.

[1] Measurements of ozone and other trace species in the European EMEP network in 2003 are presented. The European summer of 2003 was exceptionally warm, and the surface ozone data for central Europe show the highest values since the end of the 1980s. The 95th percentiles of daily maximum hourly ozone concentrations in 2003 were higher than the corresponding parameter measured in any previous year at many sites in France, Germany, Switzerland and Austria. In this paper we argue that a number of positive feedbacks between the weather conditions and ozone contributed to the elevated surface ozone. First, we calculated an extended residence time of air parcels in the atmospheric boundary layer for several sites in central Europe. Second, we show that it is likely that extensive forest fires on the Iberian Peninsula, resulting from the drought and heat, contributed to the peak ozone values in north Europe in August. Third, regional-scale model calculations indicate that enhanced levels of biogenic isoprene could have contributed up to 20% of the peak ozone concentrations. Measurements indicate elevated

Atmos. Chem. Phys., 8, 2133–2150, 2008
www.atmos-chem-phys.net/8/2133/2008/

Air pollution during the 2003 European heat wave as seen by MOZAIC airliners

M. Tressol[1], C. Ordonez[1], R. Zbinden[1], J. Brioude[2], V. Thouret[1], C. Mari[1], P. Nedelec[1], J.-P. Cammas[1], H. Smit[3], H.-W. Patz[3], and A. Volz-Thomas[3]

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[2]Chemical Sciences Division, Earth System Research Laboratory, NOAA, Boulder, Colorado, USA
[3]Institut für Chemie und Dynamik der Geosphäre II: Troposphäre, Forschungszentrum Jülich, Jülich, Germany

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Revised: 4 March 2008 – Accepted: 14 March 2008 – Published: 15 April 2008

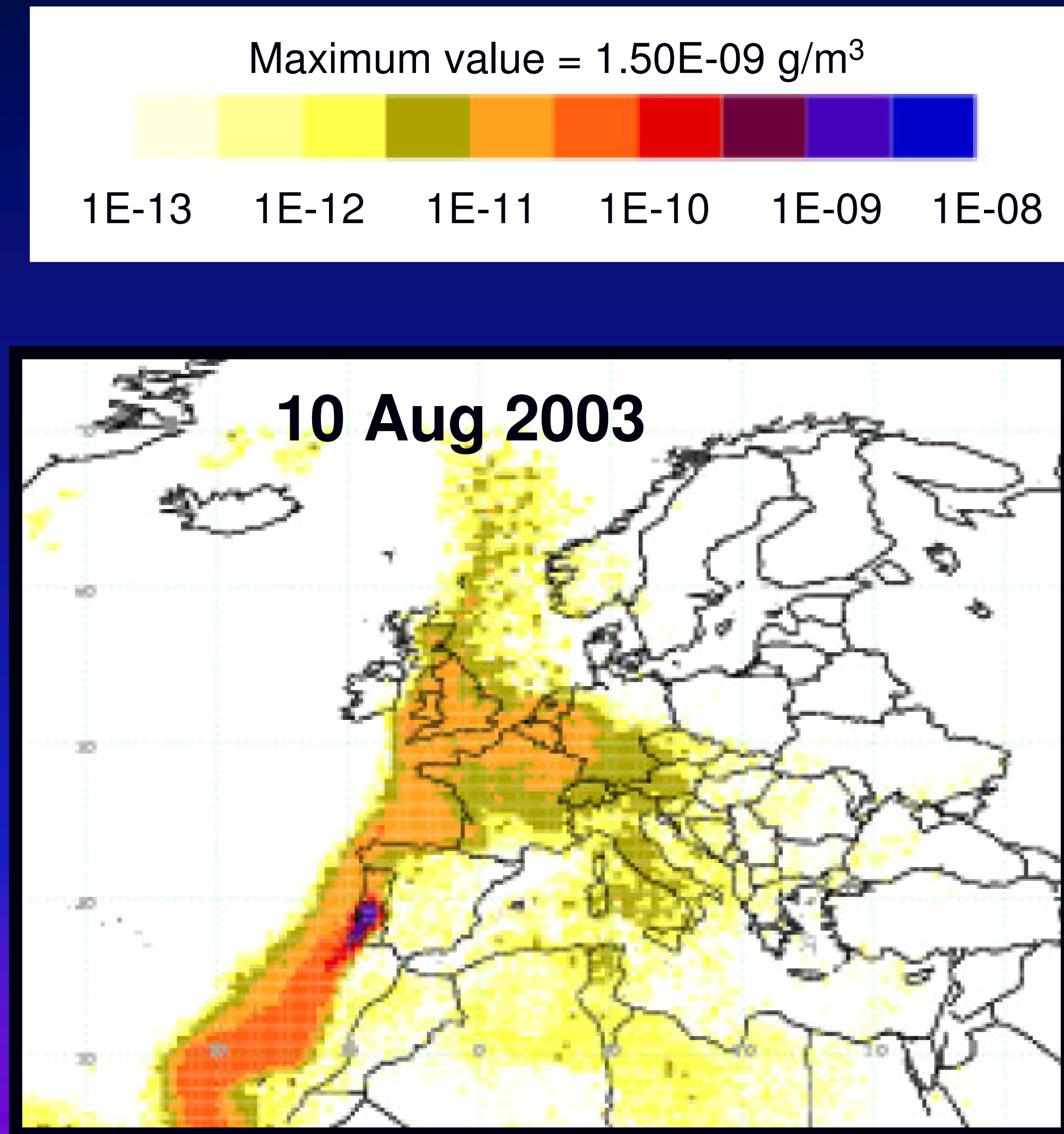
Abstract. This study presents an analysis of both MOZAIC profiles above Frankfurt and Lagrangian dispersion model simulations for the 2003 European heat wave. The comparison of MOZAIC measurements in summer 2003 with the 11-year MOZAIC climatology reflects strong temperature anomalies (exceeding 4°C) throughout the lower troposphere during the whole heat wave. European anthropogenic emissions present the strongest contribution to the measured CO levels in the lower troposphere (near 30%). This source is followed by Portuguese forest fires which affect the lower troposphere after 6 August 2003 and even the PBL around 10 August 2003. The averaged biomass burning contribution reaches

Simulation of forest fire impact at surface (0-100 m)

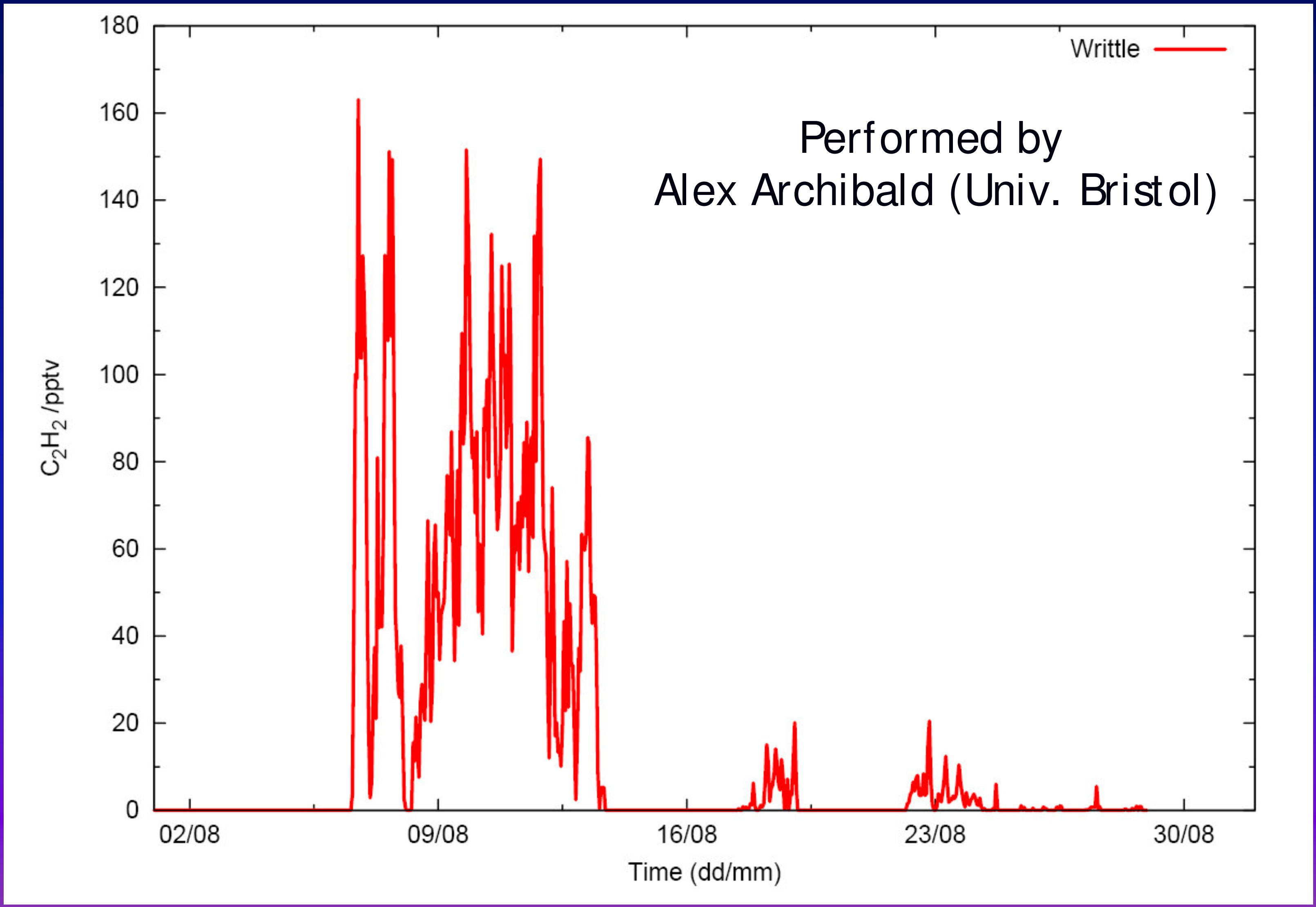
Met Office's NAME model

Performed by
Alex Archibald
(Univ. Bristol)

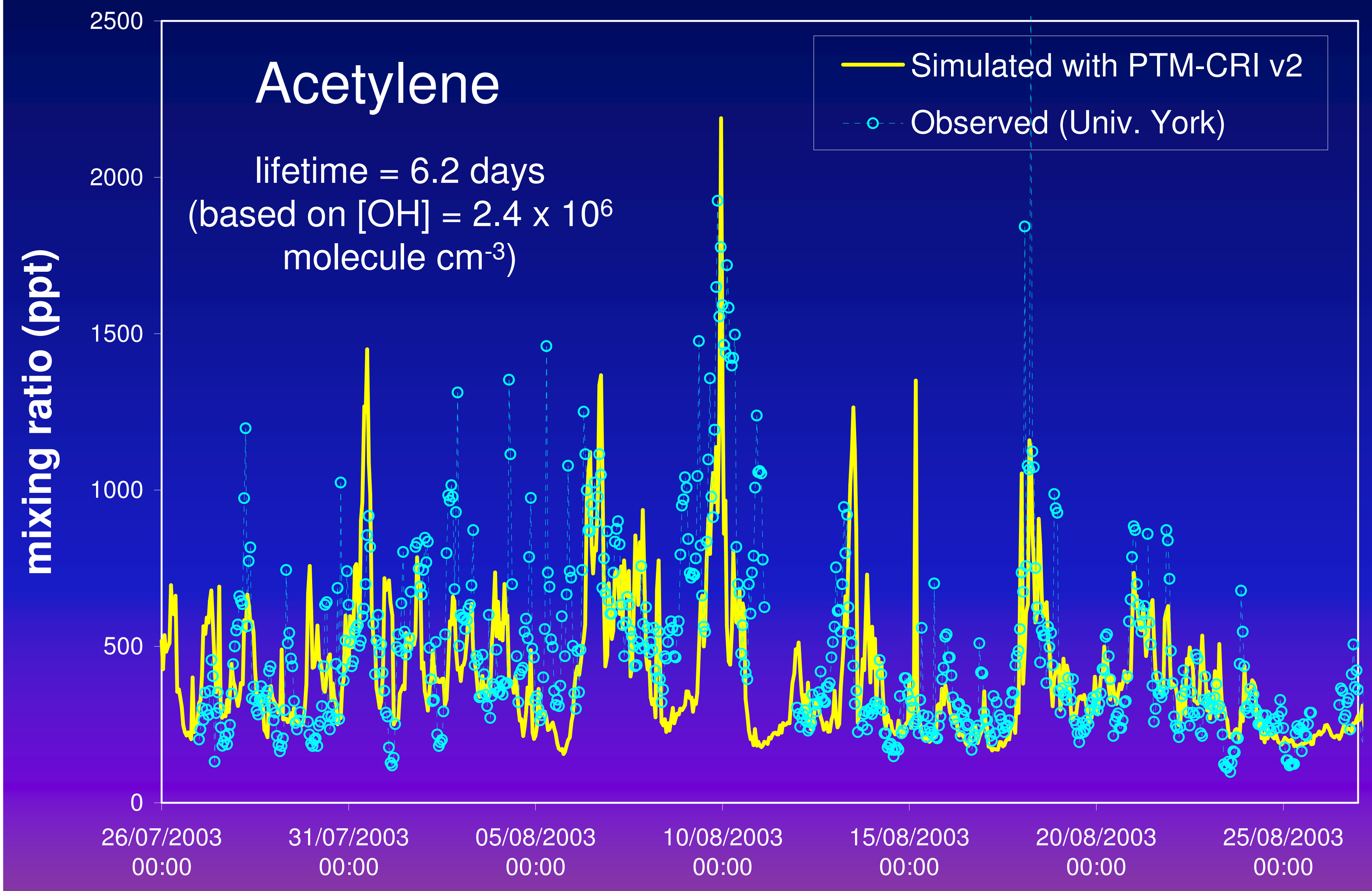
Impact at Writtle
7-13 August



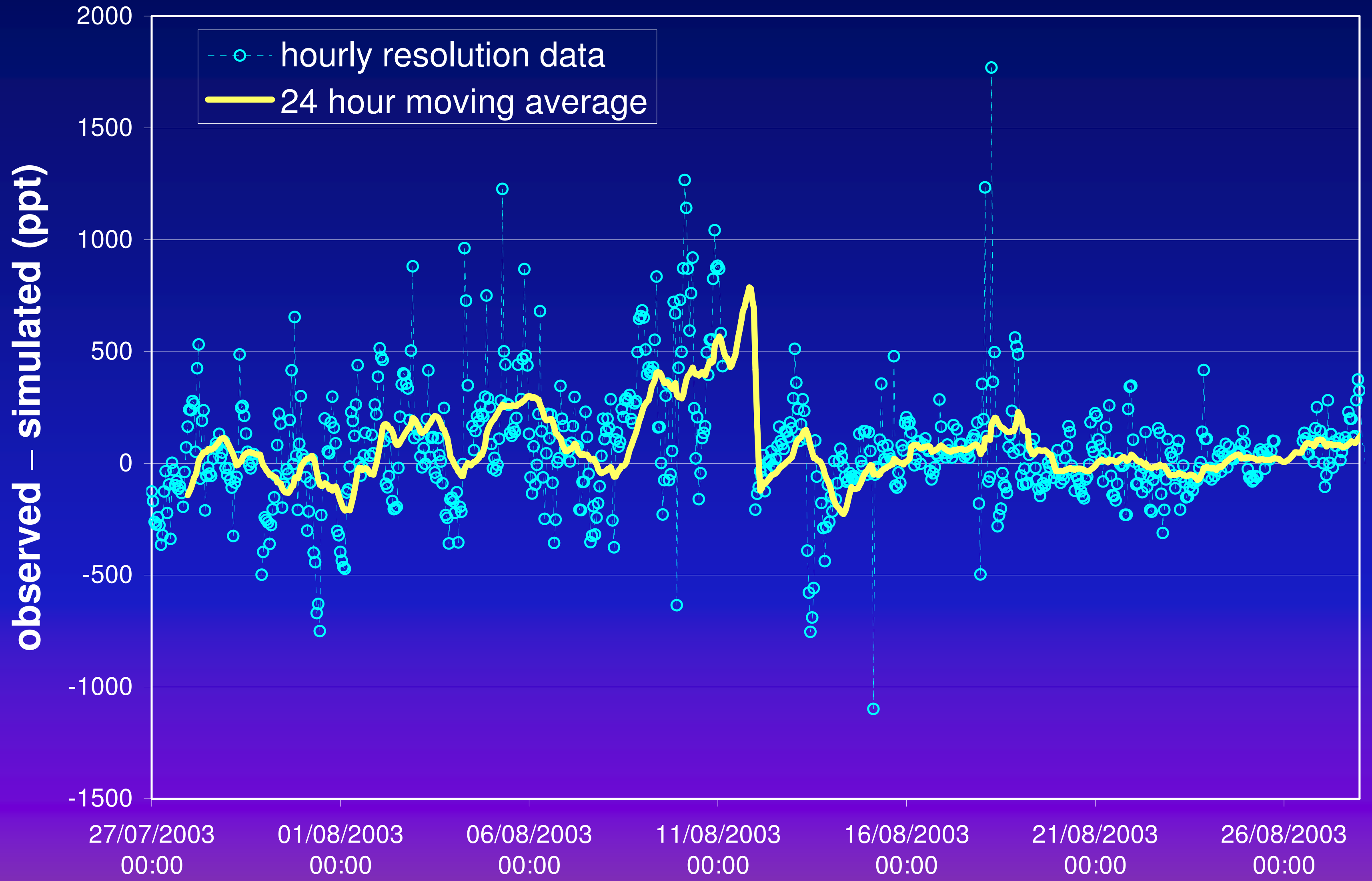
NAME simulation of acetylene from Portuguese forest fires arriving at TORCH-2003 campaign site



Comparison of PTM simulated and observed acetylene in TORCH campaign, both at hourly resolution



Difference between observed and PTM simulated acetylene in TORCH campaign



Acknowledgements

- Steve Utembe (Univ. Bristol) – PTM calculations
- Dick Derwent (rdscientific) - PTM
- Garry Hayman (NPL) – PTM/ biogenic emissions
- TORCH partners, in particular Ally Lewis, Jim Hopkins and Jacqui Hamilton (Univ. York) – hydrocarbon measurements
- Alex Archibald (Univ. Bristol) – NAME simulations

Comparison of PTM simulated and observed foraldehyde in TORCH campaign, both at hourly resolution