Chemical equation set and complete figures set

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Table 1: Reaction added to the MECCA submodel in EMAC .

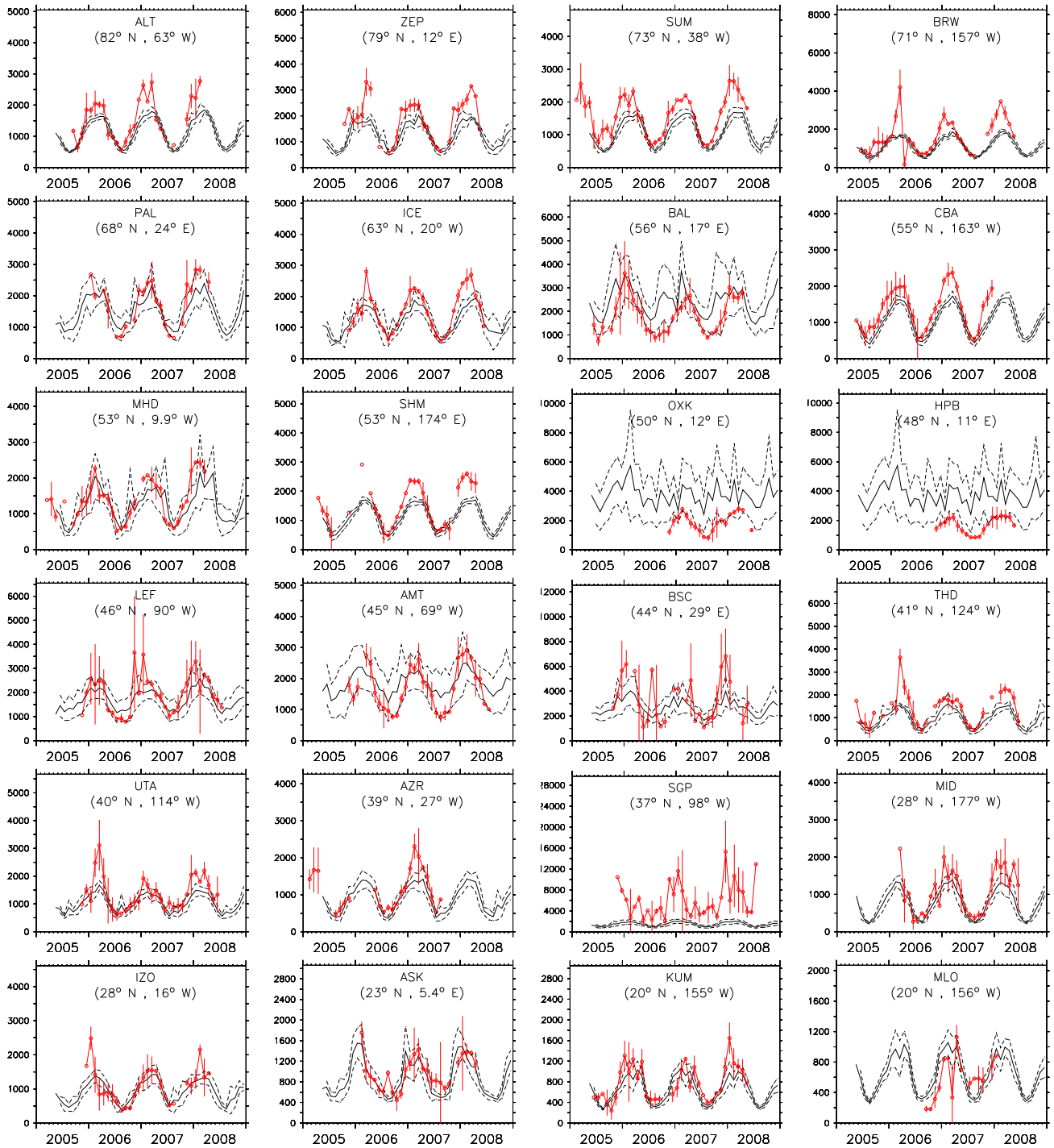
reaction	rate coefficient	reference/notes
$OH + C_4H_{10} \rightarrow HCHO + 0.4365\ CH_3CHO + 0.4365\ PA + 4.254\ PINKO_2$	$1.69 \times 10^{-17} * T^2 * e^{(145/T)}$	a, b
$CL + C_4H_{10} \rightarrow HCHO + 0.3575\ CH_3CHO + 0.3575\ PA + 4.57\ PINKO_2$	2.18×10^{-10}	a, b
$NO_3 + C_4H_{10} \rightarrow HCHO + 0.4365\ CH_3CHO + 0.4365\ PA + 4.2524\ PINKO_2$	$2.76 \times 10^{-12} * e^{(-3279/T)}$	c
$OH + IC_4H_{10} \rightarrow .206\ PrO_2 + .794\ CH_3COCH_3 + .794\ CH_3O_2 + 1.206\ PINKO_2$	$1.16 \times 10^{-17} * T^2 * e^{(225/T)}$	a, b
$CL + IC_4H_{10} \rightarrow 0.564\ PrO_2 + 0.436\ CH_3COCH_3 + 0.436\ CH_3O_2 + 1.564\ PINKO_2$	1.43×10^{-10}	a, b
$NO_3 + IC_4H_{10} \rightarrow 0.206\ PrO_2 + 0.794\ CH_3COCH_3 + 0.794\ CH_3O_2 + 1.206\ PINKO_2$	1.06×10^{-16}	c
$OH + C_5H_{12} \rightarrow 1.4765\ HCHO + 0.349\ CH_3CHO + 0.1745\ EtO_2 + 6.302\ PINKO_2$	$2.44 \times 10^{-17} * T^2 * e^{(183/T)}$	a, b
$CL + C_5H_{12} \rightarrow 1.67\ HCHO + 0.220\ CH_3CHO + 0.11\ EtO_2 + 6.56\ PINKO_2$	2.80×10^{-10}	a, b
$NO_3 + C_5H_{12} \rightarrow 1.4765\ HCHO + 0.349\ CH_3CHO + 0.1745\ EtO_2 + 6.302\ PINKO_2$	8.7×10^{-17}	c
$OH + IC_5H_{12} \rightarrow 0.087\ HCHO + 0.384\ CH3CHO + 0.297\ PrO_2 + 0.616\ CH_3COCH_3 + 0.616\ EtO_2 + 1.435\ PINKO_2$	3.70×10^{-12}	a, b
$CL + IC_5H_{12} \rightarrow 0.408\ HCHO + 0.750\ CH3CHO + 0.342\ PrO_2 + 0.250\ CH_3COCH_3 + 0.250\ EtO_2 + 3.04\ PINKO_2$	2.20×10^{-10}	a, b
$NO_3 + IC_5H_{12} \rightarrow 0.087\ HCHO + 0.384\ CH3CHO + 0.297\ PrO_2 + 0.616\ CH_3COCH_3 + 0.616\ EtO_2 + 1.435\ PINKO_2$	1.62×10^{-16}	c
$PINKO_2 + NO \rightarrow 0.95\ NO_2 + 0.475\ HO_2 + 0.475\ PINK + 0.05\ PINKNO_3$	$\left(2.54 * e^{(360./T)} + 8.10 * e^{(270./T)}\right) \times 10^{-12}/2$	h
$PINKO_2 + CH_3O_2 \rightarrow 0.5\ HO_2 + 0.335\ CH_3OH + 0.665\ HCHO + 0.335\ HO_2$	$2. \times 10^{-12}$	h
$PINKO_2 + HO_2 \rightarrow PINKOOH$	$\left(4.30 * e^{(1040./T)} + 2.91 * e^{(1300./T)}\right) \times 10^{-13}/2$	h
$PINK + OH \rightarrow CO_2$	2×10^{-11}	d
$PINK + hv \rightarrow HO_2$	J-CH3CHO	d
$PINKNO_3 + OH \rightarrow NO_2$	$5. \times 10^{-12}$	
$PINKNO_3 + hv \rightarrow NO_2$	3.7*J-PAN	e
$PINKOOH + hv \rightarrow OH + 0.5\ HO_2$	J-CH3OOH	f
$PINKOOH + OH \rightarrow PINKO_2$	$1.90 \times 10^{-12} * e^{(190./T)}$	a, b
$PINKOOH + OH \rightarrow OH$	$2. \times 10^{-11}$	g

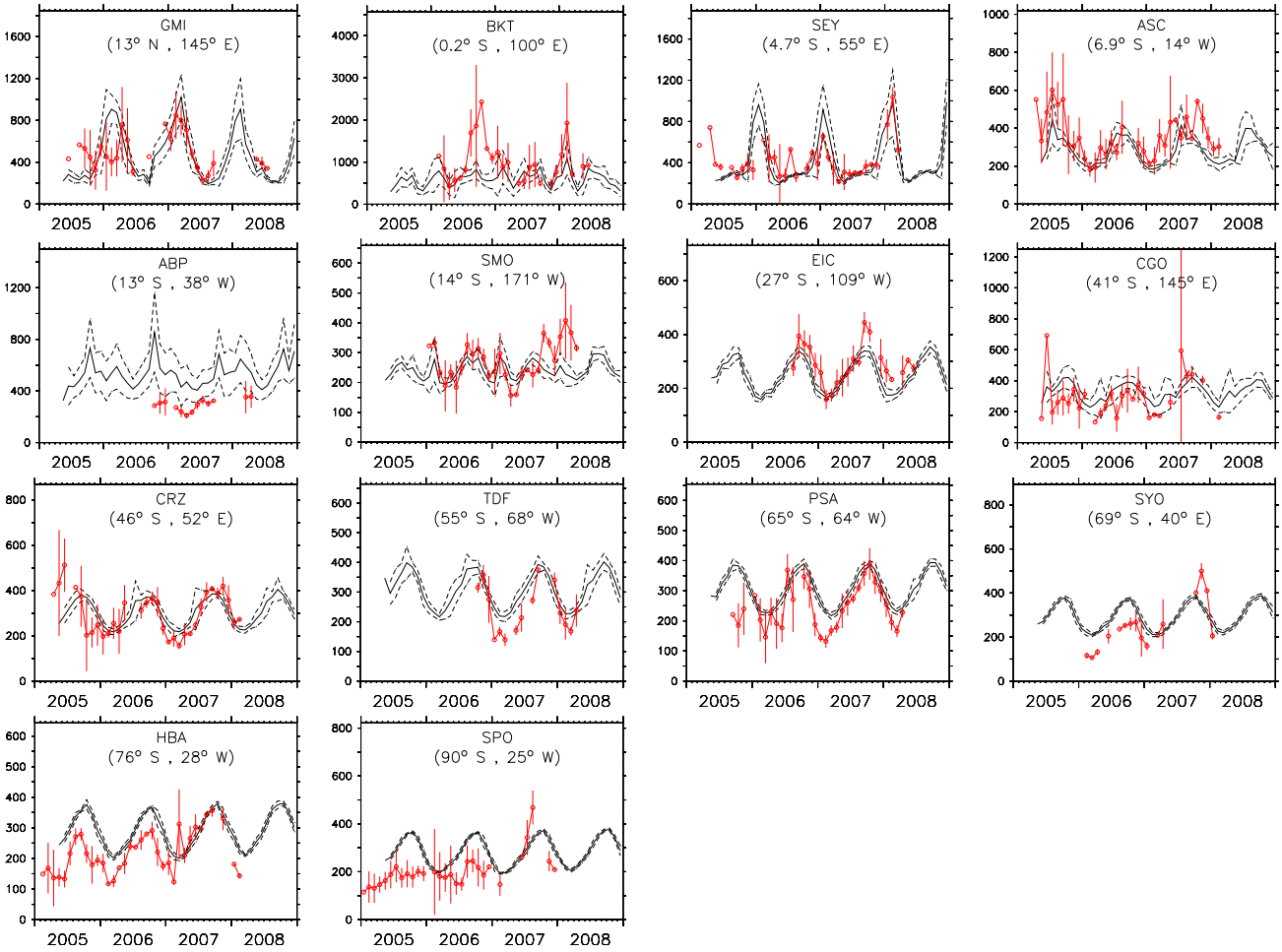
[a] Saunders et al. (1997a)
[b] Saunders et al. (1997b)
[c] Atkinson and Arey (2003), branching ratio like the OH reaction
[d] as general aldehyde
[e] photolysis scale with PAN photolysis rate
[f] photolysis scale with CH_3OOH photolysis rate
[g] representative for the H-abstraction of these peroxides
[h] average between the reactions of the two different peroxides isomers

Model-observation comparison

Ethane (C_2H_6)

Comparison of simulated and observed C_2H_6 mixing ratios in nmol/mol for some selected location (ordered by latitude). The red line and the bars represent the monthly average and the standard deviation (w.r.t. time) of the measurements in the region. No instrumental error has been included in this standard deviation. The simulated monthly average is indicated in the black line and the corresponding simulated standard deviation (w.r.t. time) by the dashed line.

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EIC
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TDF
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PSA
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SYO
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HBA
(76° S , 28° W)
SPO
(90° S , 25° W)
2005
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2007
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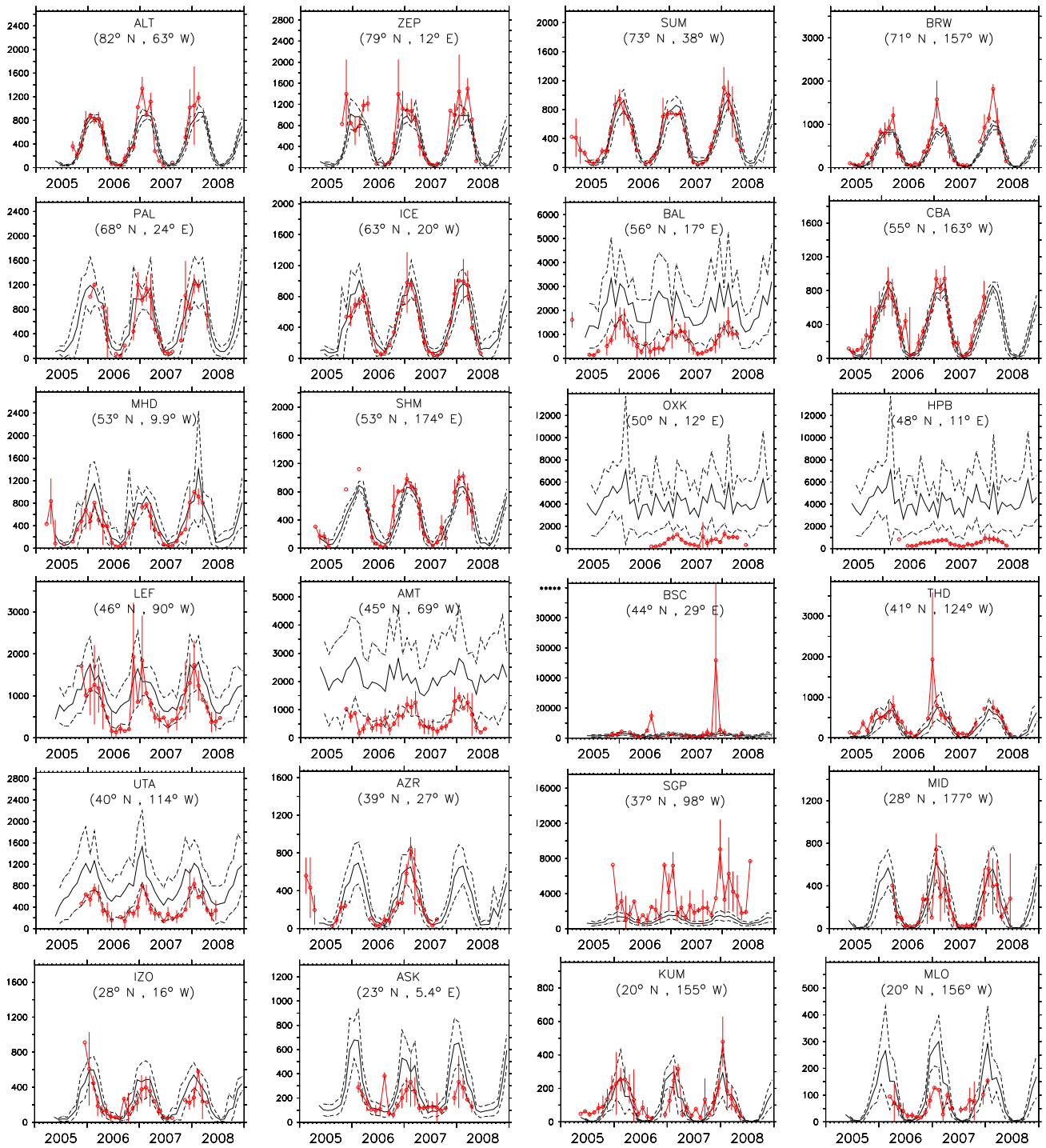
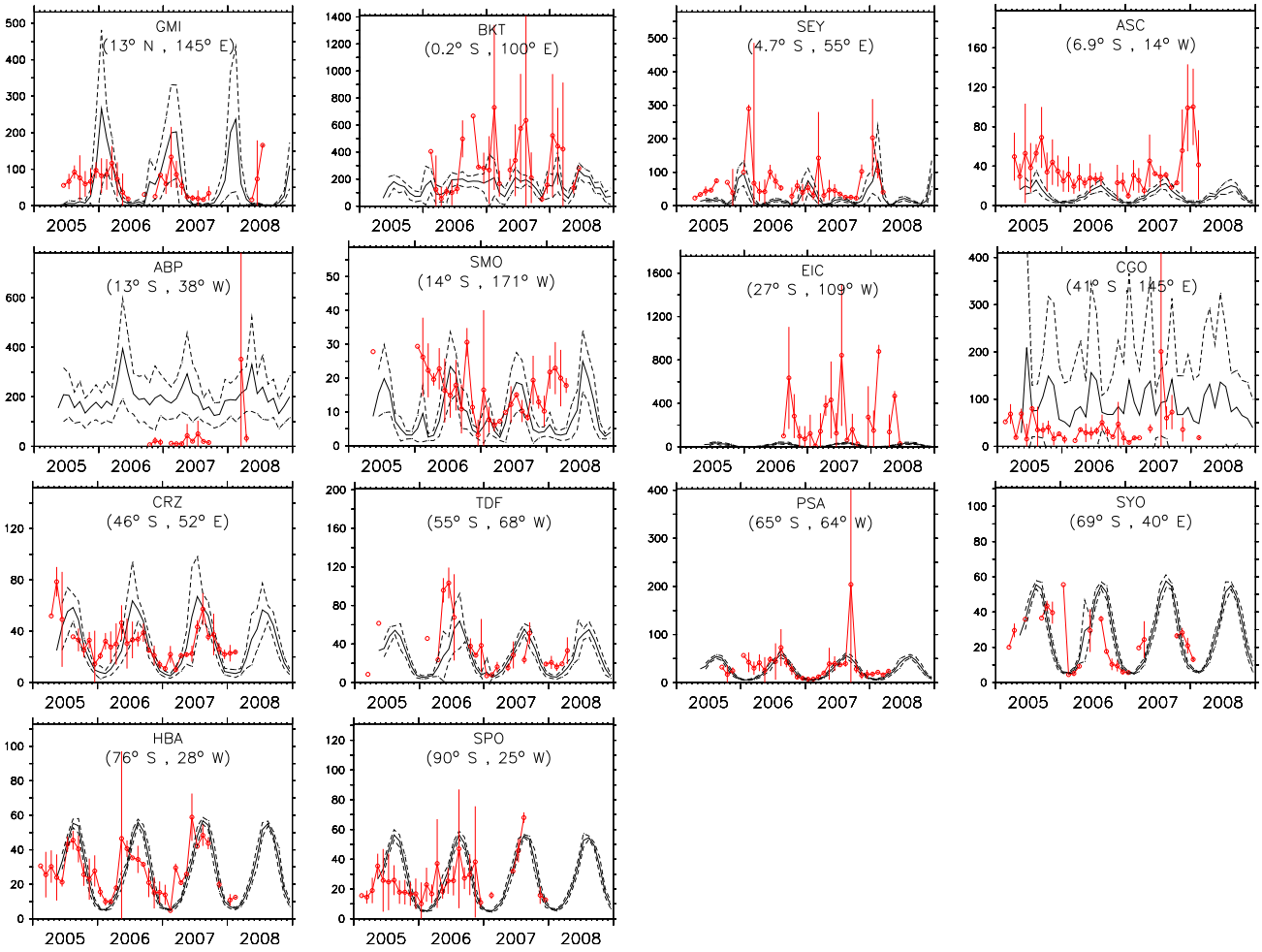
Propane (C_3H_8)

Comparison of simulated and observed C_3H_8 mixing ratios in nmol/mol for some selected location (ordered by latitude). The red line and the bars represent the monthly average and the standard deviation (w.r.t. time) of the measurements in the region. No instrumental error has been included in this standard deviation. The simulated monthly average is indicated in the black line and the corresponding simulated standard deviation (w.r.t. time) by the dashed line.

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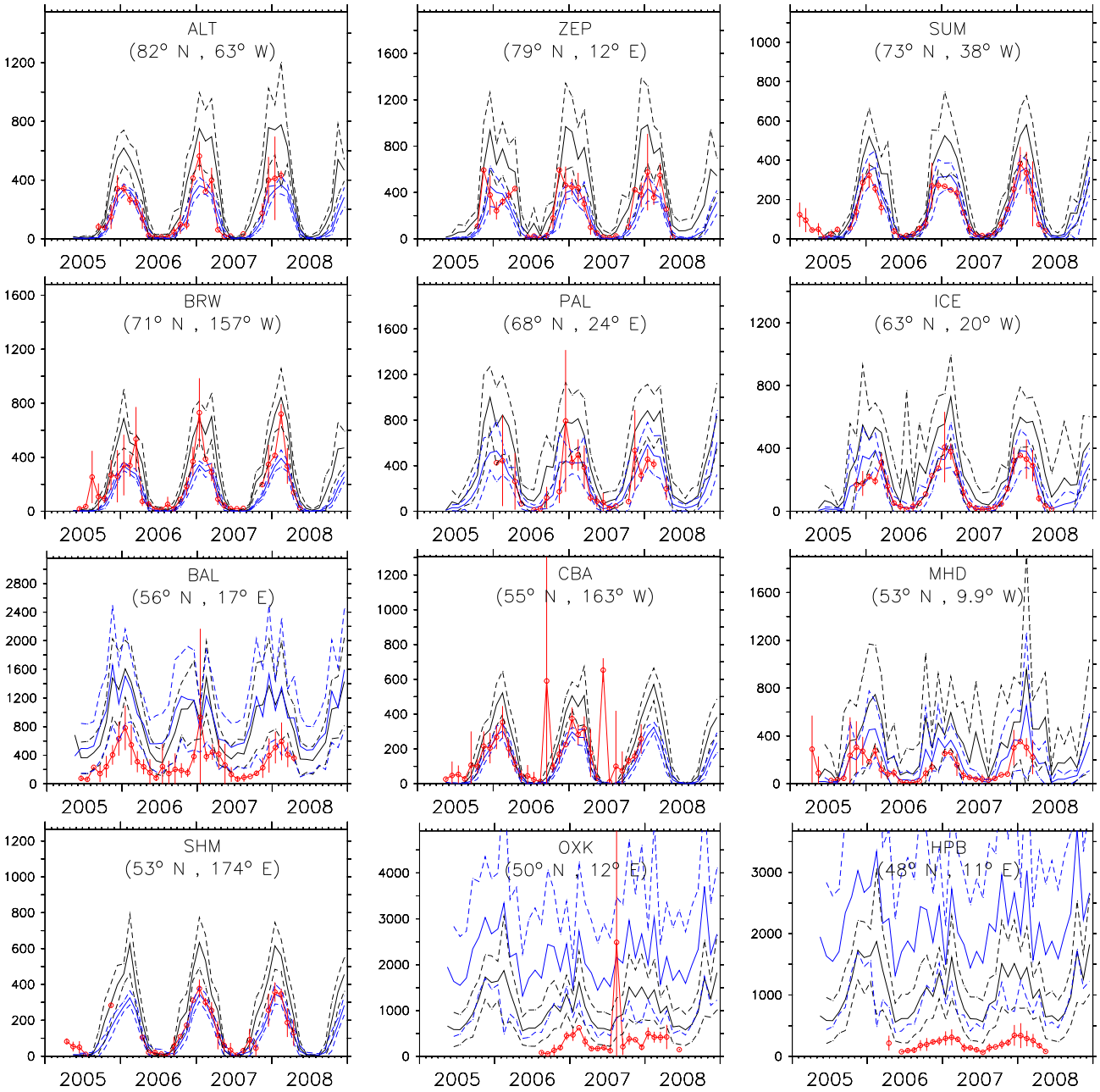
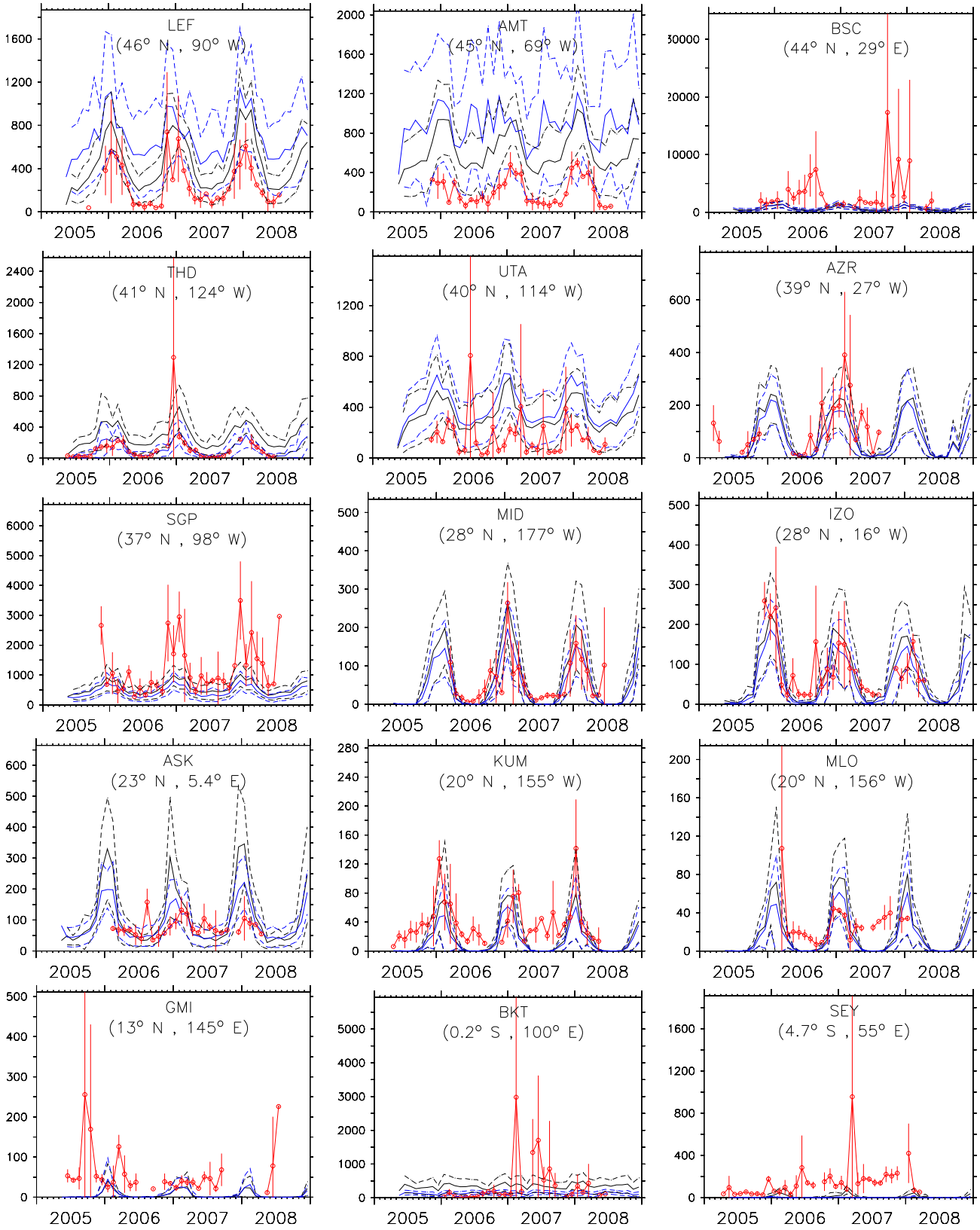
Butane (C_4H_{10})

Comparison of simulated and observed C_4H_{10} mixing ratios in nmol/mol for some selected location (ordered by latitude). The red line and the bars represent the monthly average and the standard deviation (w.r.t. time) of the measurements in the region. No instrumental error has been included in this standard deviation. The simulated monthly average is indicated in the solid line and the corresponding simulated standard deviation (with respect to time) by the dashed line. The black and blue colors denote results from simulation *E1* and *E2*, respectively.

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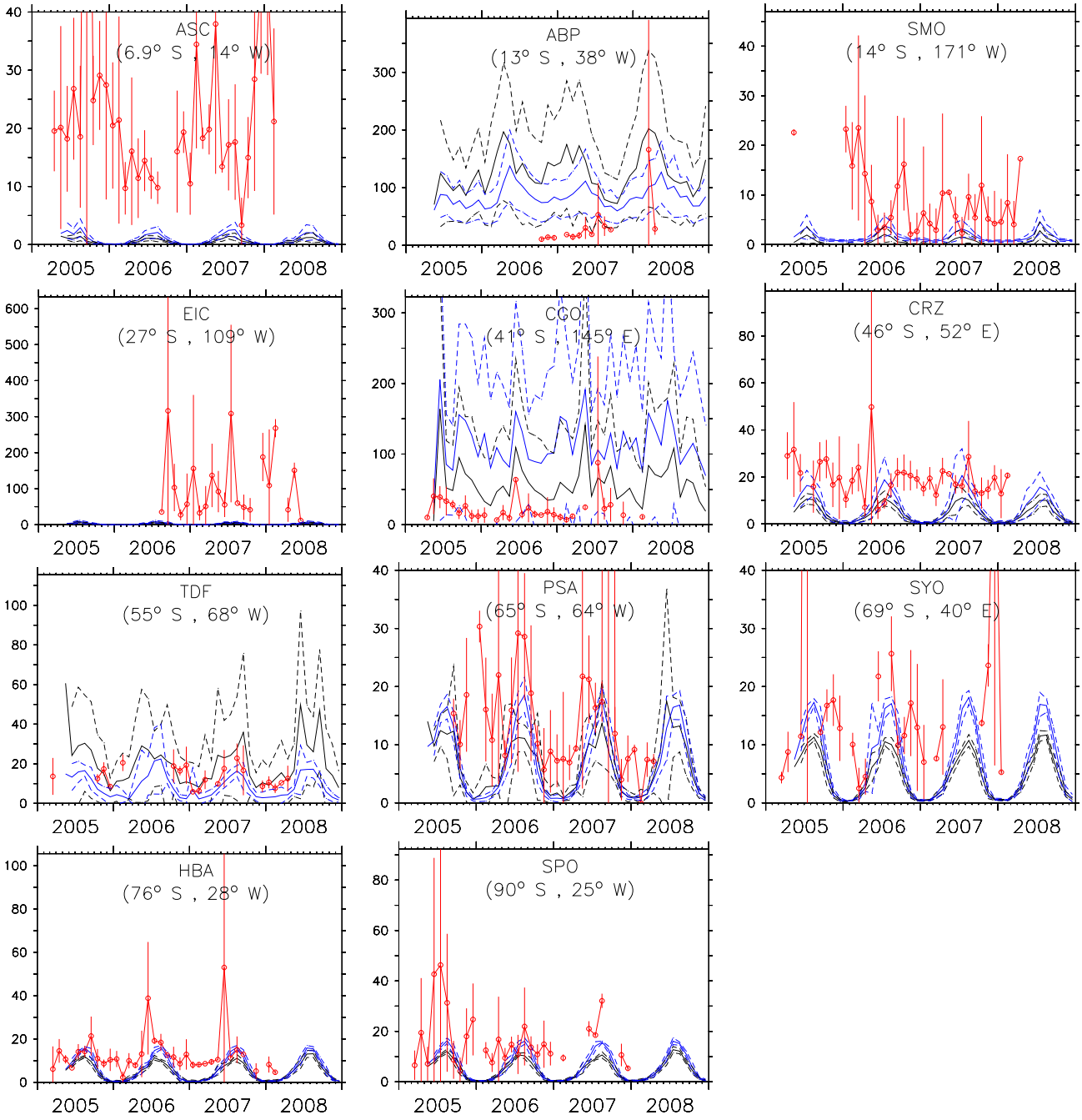
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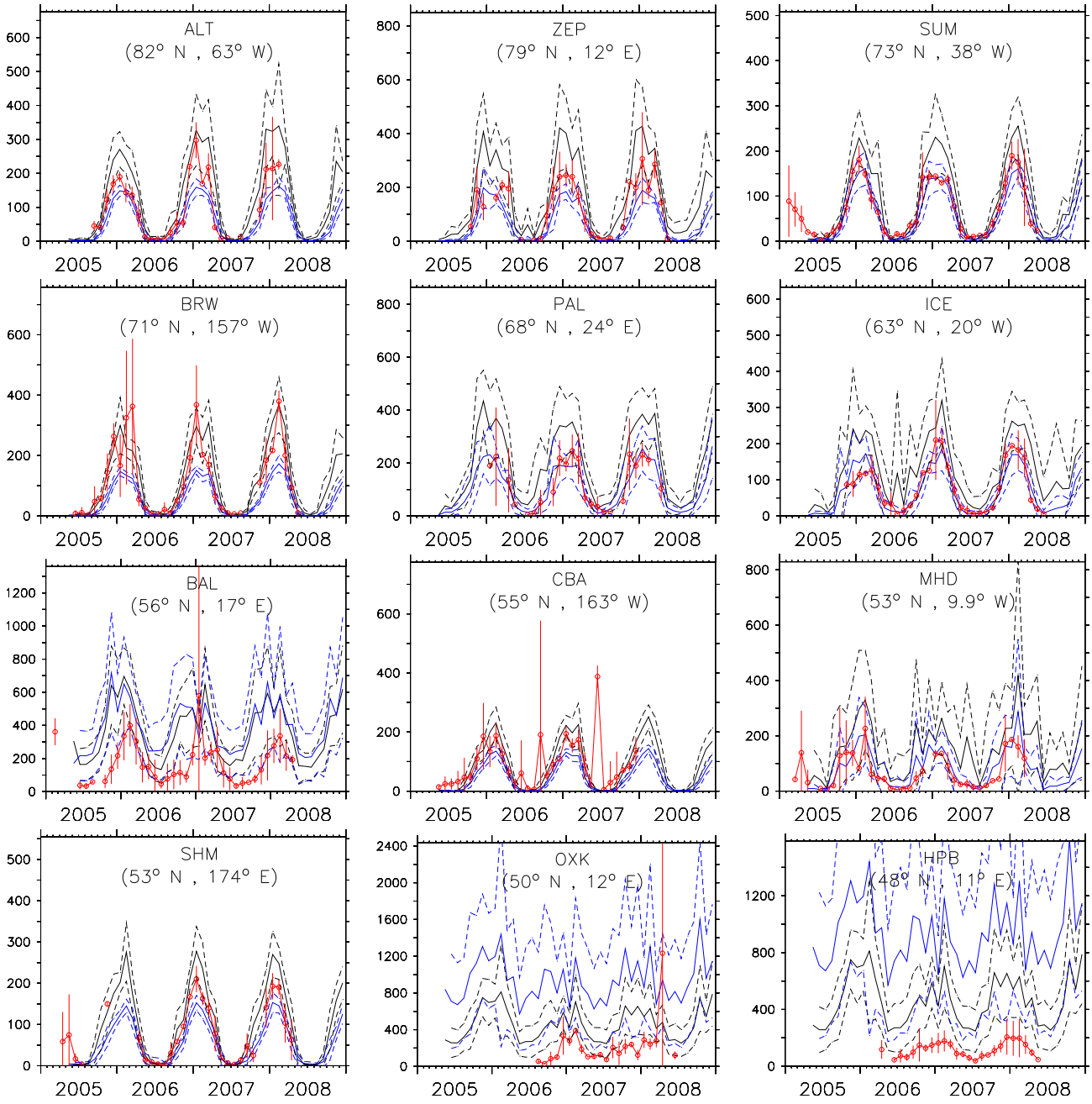
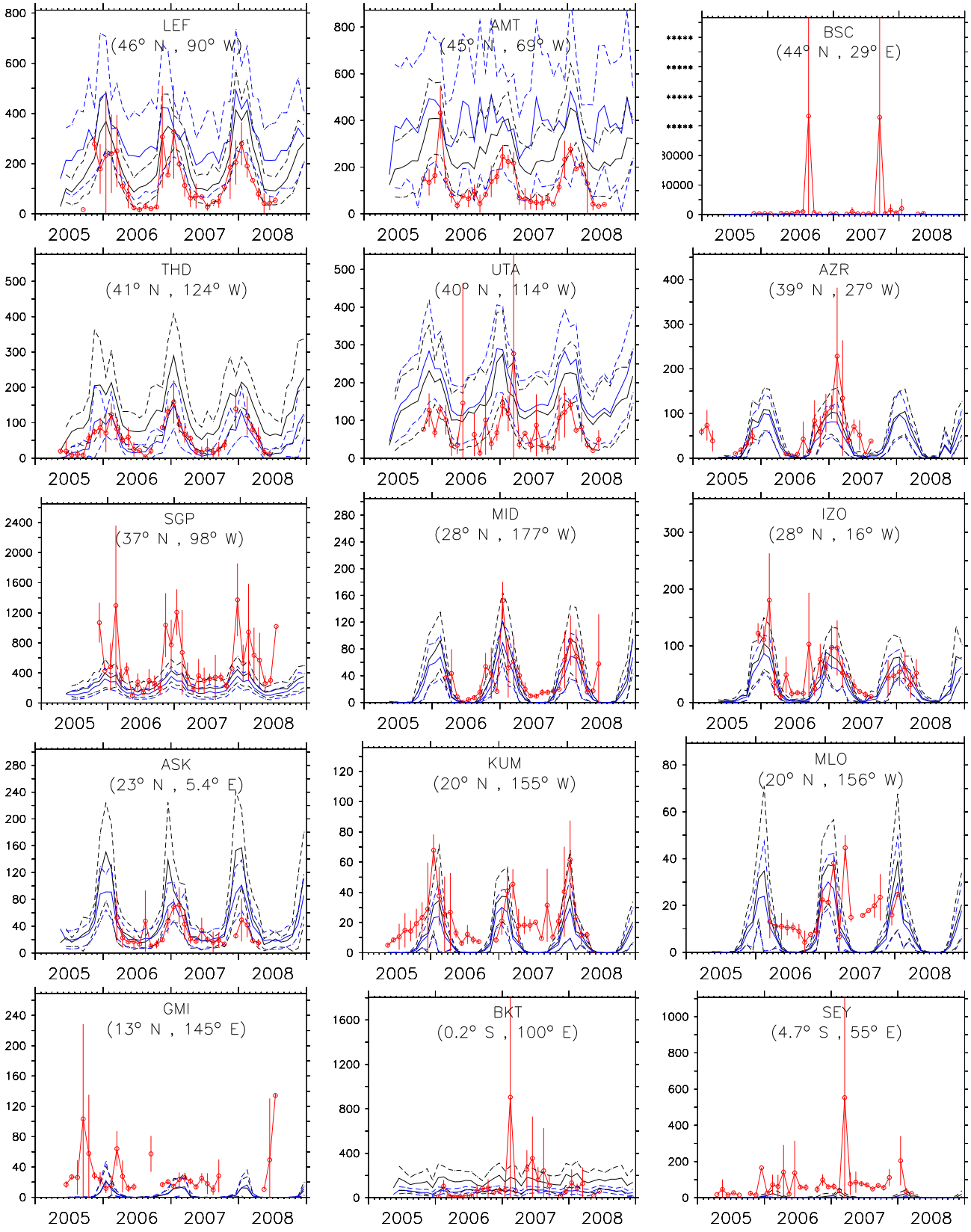
Isobutane ($I-C_4H_{10}$)

Comparison of simulated and observed $I-C_4H_{10}$ mixing ratios in nmol/mol for some selected location (ordered by latitude). The red line and the bars represent the monthly average and the standard deviation (w.r.t. time) of the measurements in the region. No instrumental error has been included in this standard deviation. The simulated monthly average is indicated in the solid line and the corresponding simulated standard deviation (with respect to time) by the dashed line. The black and blue colors denote results from simulation *E1* and *E2*, respectively.

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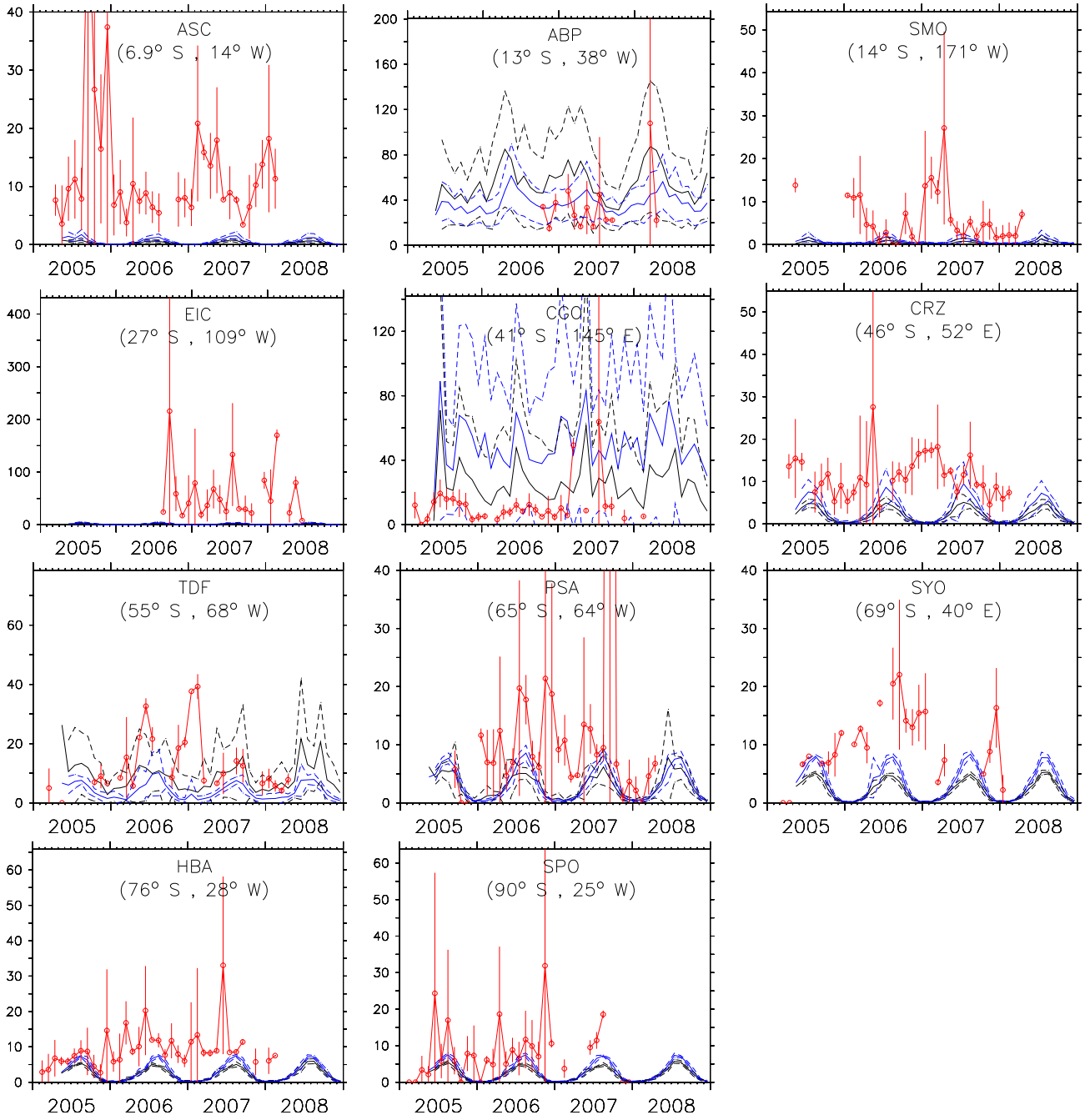
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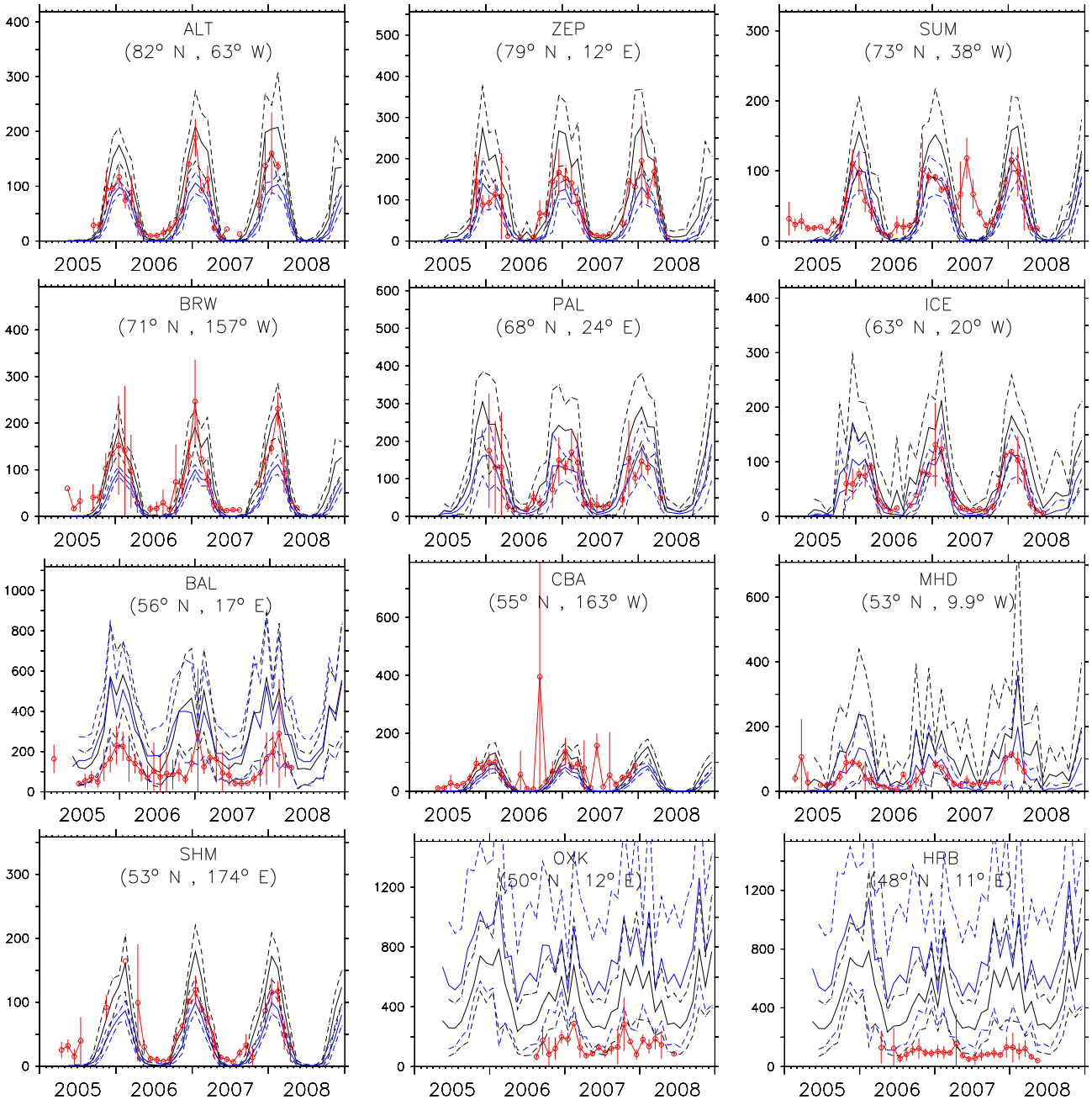
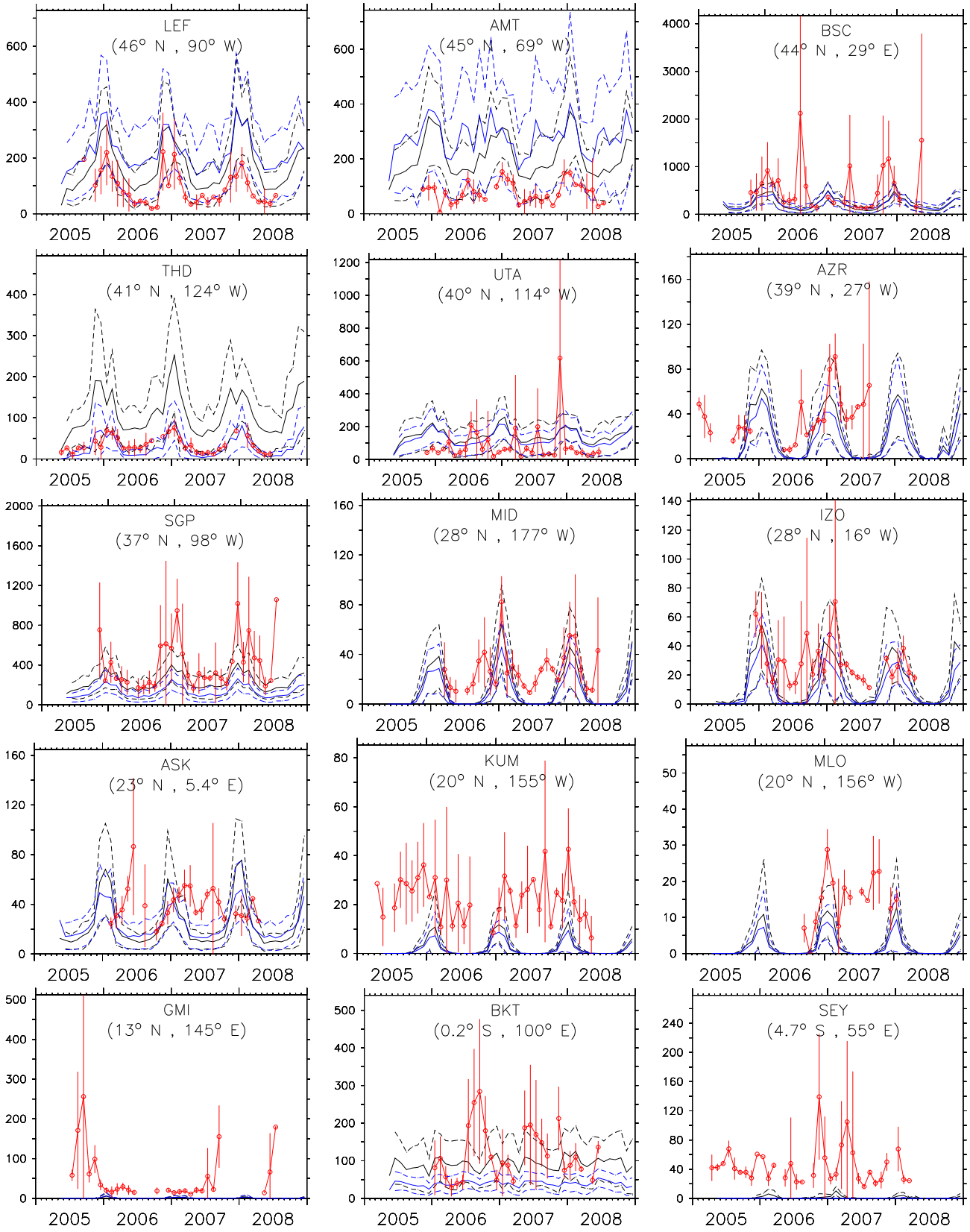
Pentane (C_5H_{12})

Comparison of simulated and observed C_5H_{12} mixing ratios in nmol/mol for some selected location (ordered by latitude). The red line and the bars represent the monthly average and the standard deviation (w.r.t. time) of the measurements in the region. No instrumental error has been included in this standard deviation. The simulated monthly average is indicated in the solid line and the corresponding simulated standard deviation (with respect to time) by the dashed line. The black and blue colors denote results from simulation *E1* and *E2*, respectively.

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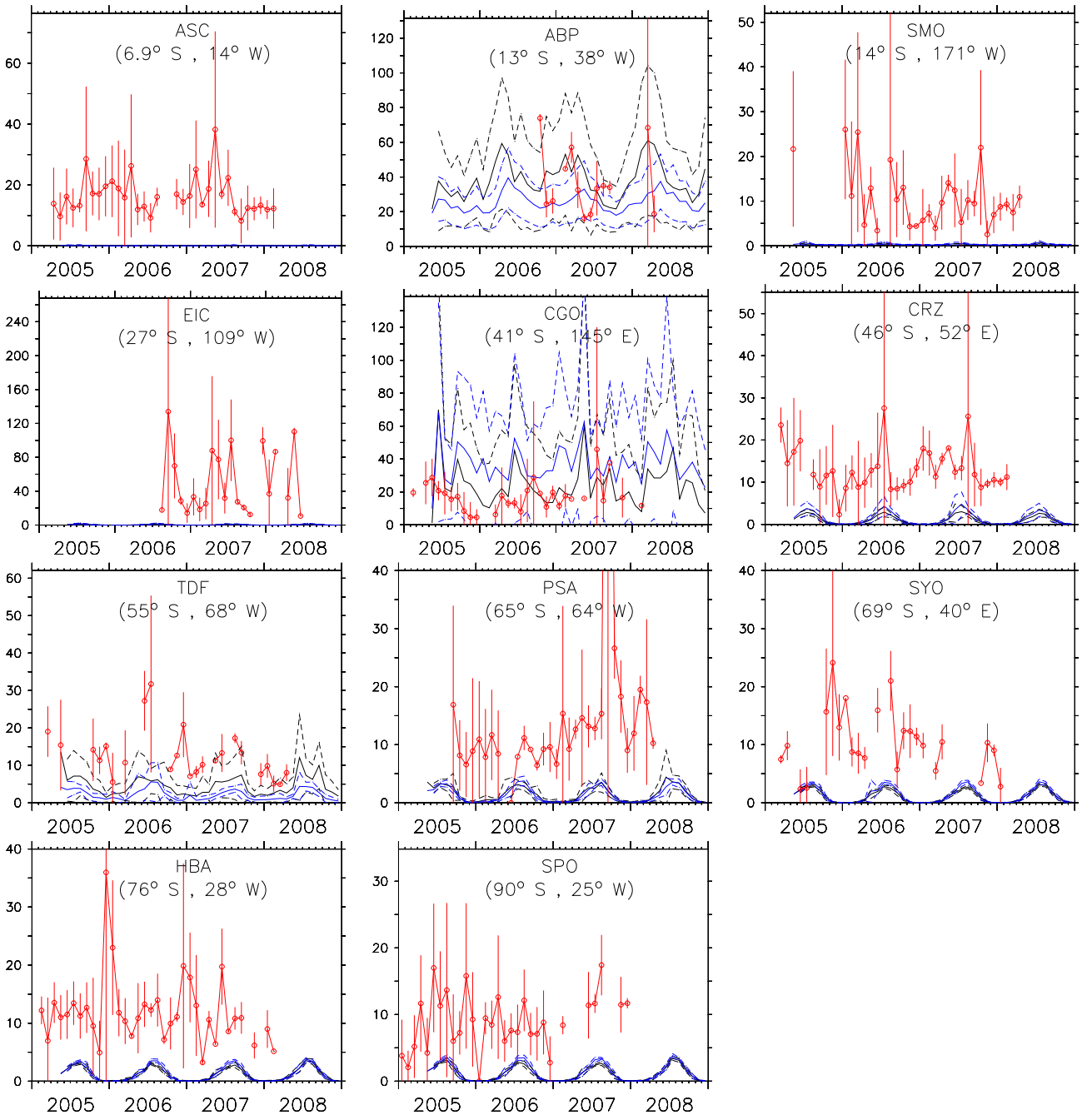
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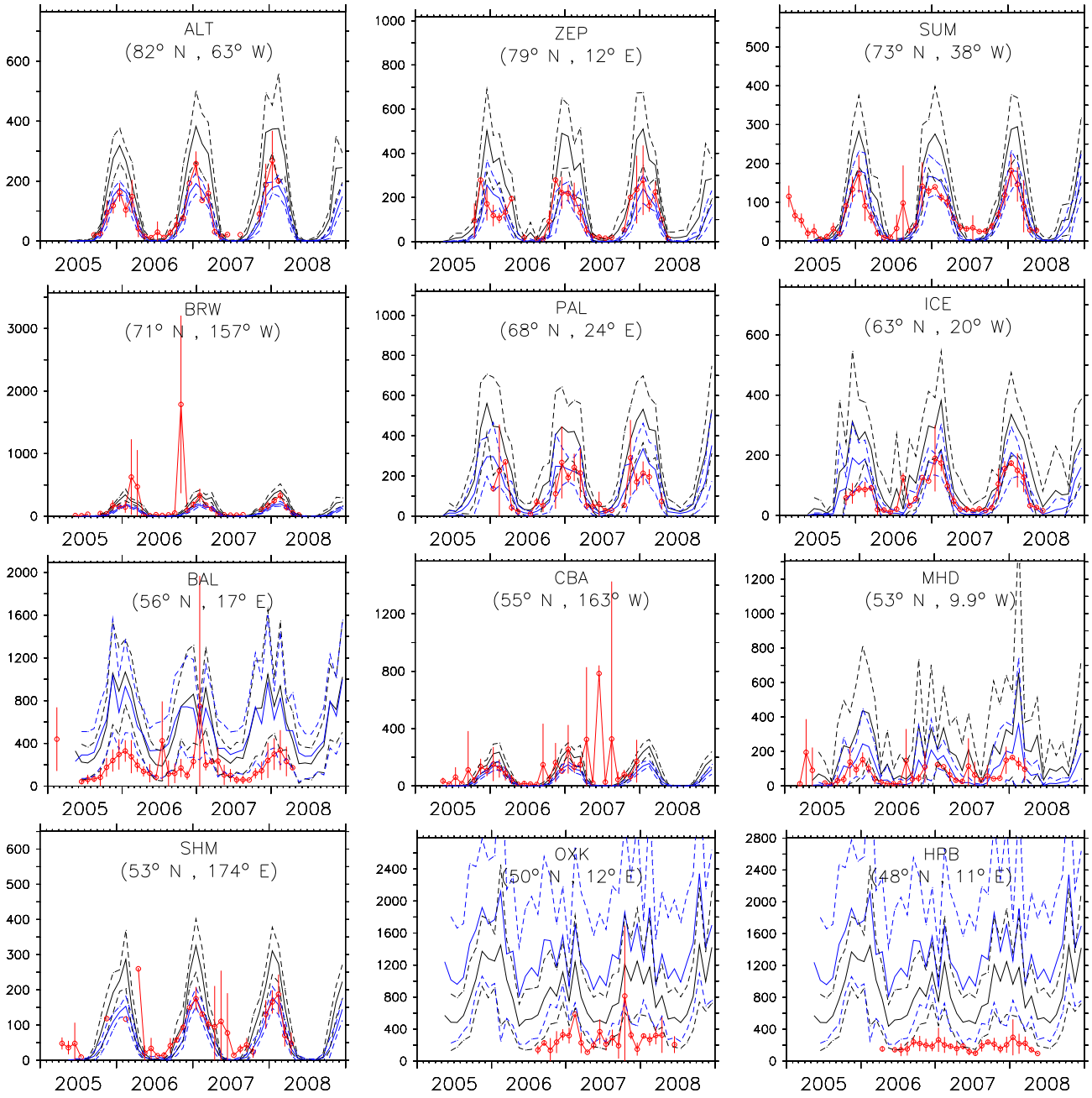
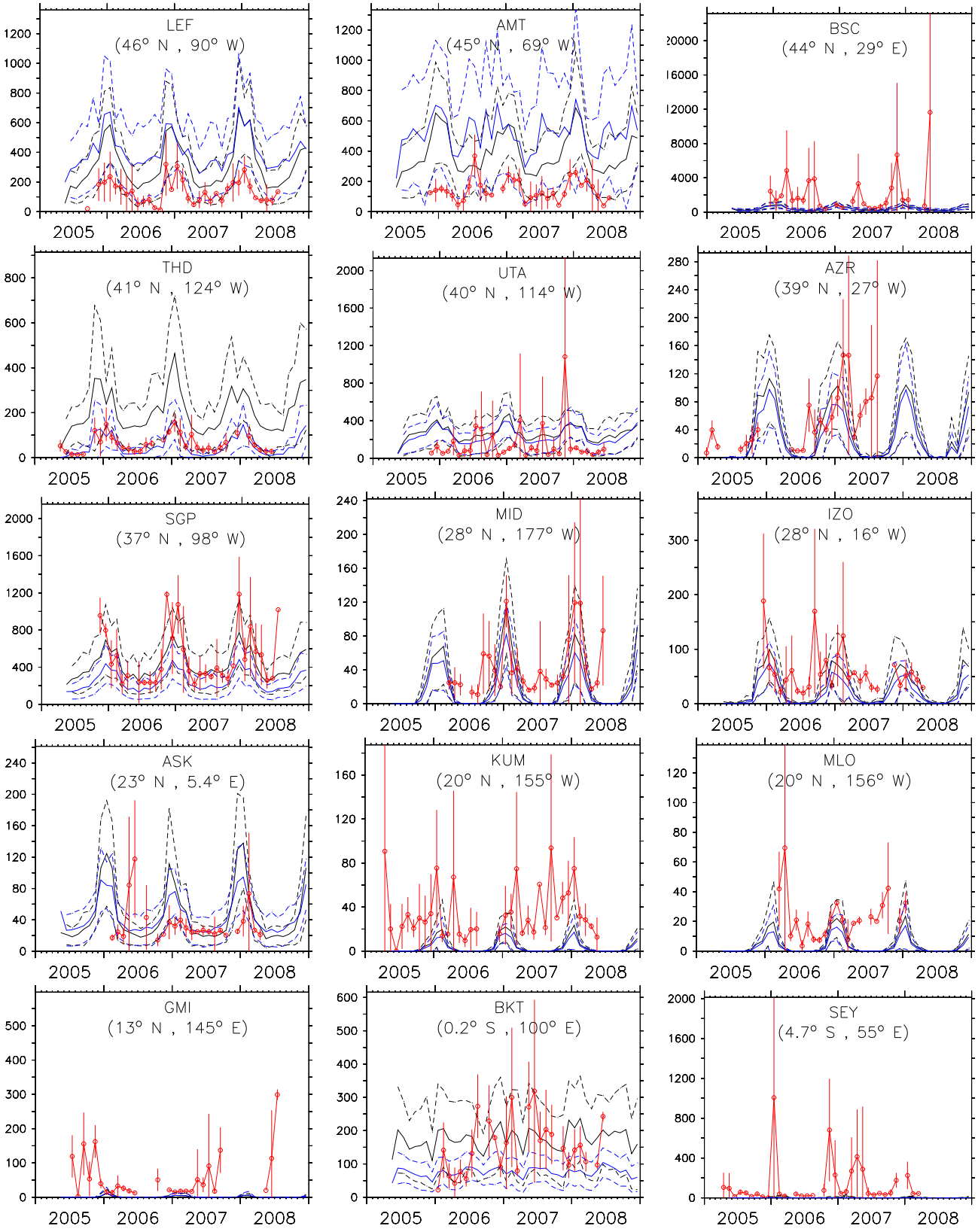
Isopentane ($I-C_5H_{12}$)

Comparison of simulated and observed $I-C_5H_{12}$ mixing ratios in nmol/mol for some selected location (ordered by latitude). The red line and the bars represent the monthly average and the standard deviation (w.r.t. time) of the measurements in the region. No instrumental error has been included in this standard deviation. The simulated monthly average is indicated in the solid line and the corresponding simulated standard deviation (with respect to time) by the dashed line. The black and blue colors denote results from simulation *E1* and *E2*, respectively.

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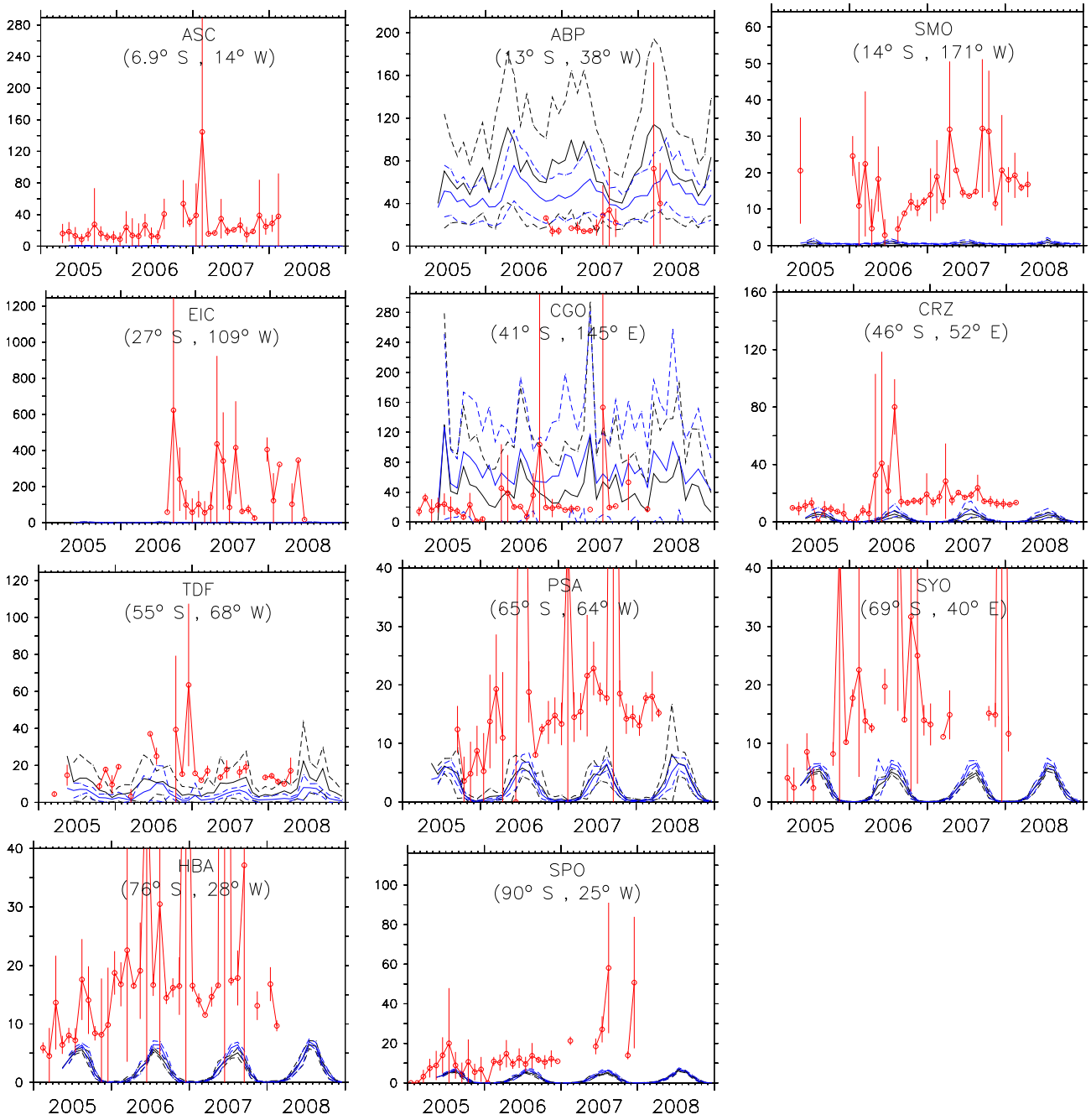
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2005
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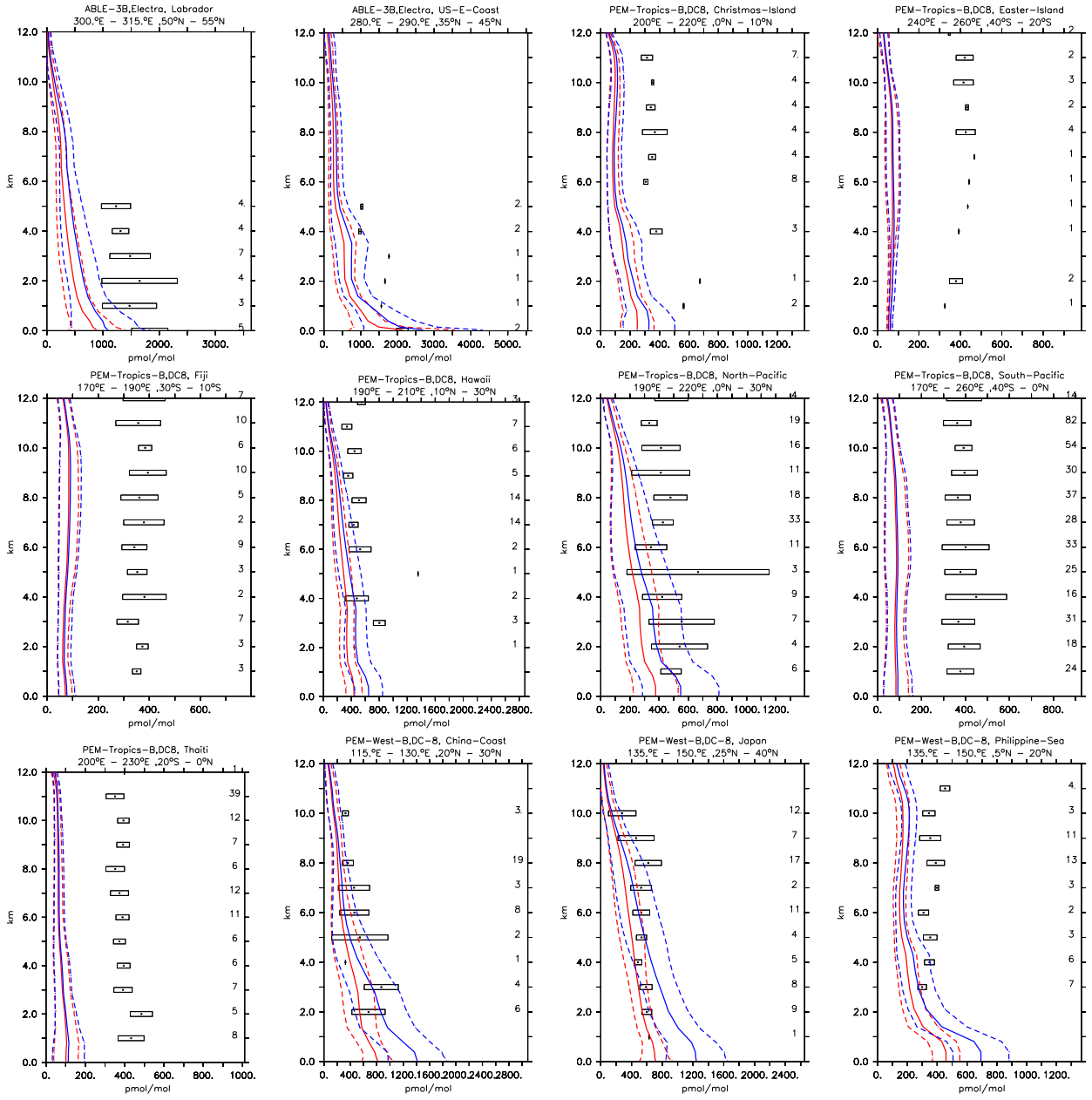
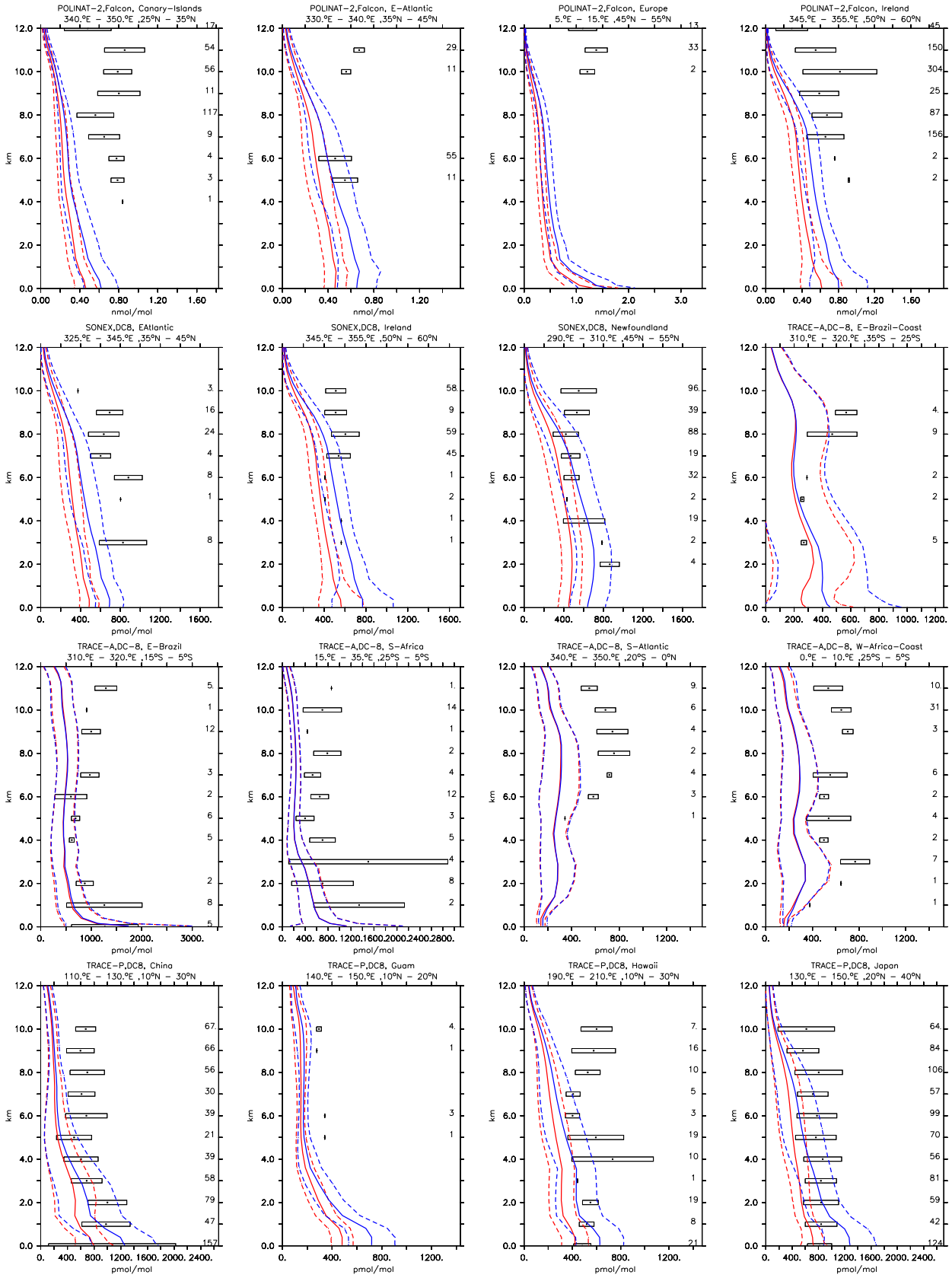
Acetone formation

Vertical profiles of CH_3COCH_3 (in pmol/mol) for some selected campaigns from Emmons et al. (2000). Asterisks and boxes represent the average and the standard deviation (with respect to space and time) of the measurements in the region, respectively. The simulated average is indicated by the solid line and the corresponding simulated standard deviation with respect to time and space by the dashed lines. On the right axis the numbers of measurements are listed. The red lines represent the simulation S1, the blue lines the simulation *E2*.

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POLINAT−2,Falcon, E−Atlantic
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POLINAT−2,Falcon, Europe
5.°E − 15.°E ,45°N − 55°N
POLINAT−2,Falcon, Ireland
345.°E − 355.°E ,50°N − 60°N
SONEX,DC8, EAtlantic
325.°E − 345.°E ,35°N − 45°N
SONEX,DC8, Ireland
345.°E − 355.°E ,50°N − 60°N
SONEX,DC8, Newfoundland
290.°E − 310.°E ,45°N − 55°N
TRACE−A,DC−8, E−Brazil−Coast
310.°E − 320.°E ,35°S − 25°S
TRACE−A,DC−8, E−Brazil
310.°E − 320.°E ,15°S − 5°S
TRACE−A,DC−8, S−Africa
15.°E − 35.°E ,25°S − 5°S
TRACE−A,DC−8, S−Atlantic
340.°E − 350.°E ,20°S − 0°N
TRACE−A,DC−8, W−Africa−Coast
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190.°E − 210.°E ,10°N − 30°N
TRACE−P,DC8, Japan
130.°E − 150.°E ,20°N − 40°N
km
nmol/mol
pmol/mol

References

Atkinson, R. and Arey, J.: Gas-Phase tropospheric chemistry of biogenic volatile compounds: a review, Atmos. Environ., 37, 197–297, 2003.

Emmons, L. K., Hauglustaine, D. A., Müller, J.-F., Carroll, M. A., Brasseur, G. P., Brunner, D., Staehelin, J., Thouret, V., and Marenco, A.: Data composites of airborne observations of tropospheric ozone and its precursors, J. Geophys. Res., 105, 20 497–20 538, 2000.

Saunders, S. M., Jenkin, M. E., Derwent, R. G., and Pilling, M. J.: Development of a Master Chemical Mechanism for Use in Tropospheric Chemistry Models, EUROTRAC Newsletter 18, 1997a.

Saunders, S. M., Jenkin, M. E., Derwent, R. G., and Pilling, M. J.: World Wide Web site of a Master Chemical Mechanism (MCM) for use in tropospheric chemistry models, Atmos. Environ., 31, 1249, http://www.chem.leeds.ac.uk/Atmospheric/MCM/-mcmproj.html, `http://www.chem.leeds.ac.uk/Atmospheric/MCM/\-mcmproj.html`, 1997b.