The implementation of an explicit gas-phase chemical scheme in TM5-MP

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with the contribution of

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Outlook

Part 1

1. Description of the new chemical scheme
2. Emissions
3. TM5MP - MOGUNTIA scheme coupling
4. TM5MP – KPP coupling

Part 2

1. Ozone evaluation
2. CO evaluation
3. Conclusions and Further work…

The MOGUNTIA chemical scheme in TM5-MP

- The MOGUNTIA chemical scheme (*Poisson et al., 2000; Myriokefalitakis et al., 2008, 2011*) is a rather explicit oxidation mechanism of Volatile Organic Compounds (VOCs) including biogenic and aromatic hydrocarbon chemistry:
  - C_1-C_3: detailed oxidation
    - *light alkanes (CH_4, C_2H_6 and C_3H_8, C_4H_{10}), light alkenes (C_2H_4 and C_3H_6)*
    - *CH_3CHO, CHOCHO, HOCHCHO, CH_3COCHO and CH_3COCH_3*
    - *Methacrolein and Methylvinyl ketone*
    - *NO_3 oxidation of aldehydes, alcohols, n-C_4H_{10}, and unsaturated hydrocarbons are also considered.*
  - $C_{(n\geq4)}$ (higher VOCs): based on n-butane oxidation
  - Isoprene: detailed oxidation
  - Terpenes: simplified chemistry based on isoprene oxidation
  - Aromatics: simplified chemistry based on $C_{(n\geq4)}$ oxidation
  - Sulphur and ammonia chemistry as well as heterogeneous reactions as in the standard CB05 scheme

VOC EMISSIONS in TM5-MP

Species	Long name	Emissions (Tg yr^{-1})
CO	Carbon Monoxide	1095.0
CH4	Methane	613.3
C_5H_8 (ISOP)	Isoprene	572.5
CH_3OH	Methanol	145.0
CH_3CHO	Acetaldehyde	132.1
$C_{10}H_{16}$ (TERP)	Terpenes	103.4
NH_3	Ammonia	95.7
NOx	Nitrogen Oxides	70.9
C_4H_{10}	Butane and higher alkanes	59.9
CH_3COCH_3 (ACET)	Acetone (includes all ketones except MEK from BB)	53.4
CH_3SCH_3 (DMS)	Dimethylsulphide (DMS)	41.2
C_3H_6	Propene	37.2
C_2H_4 (ETH)	Ethene	28.9
CH_3COOH (MCOOH)	Acetic acid	26.3
CH_3CH_2OH (ETHOH)	Ethanol	26.0
C_7H_8 (AROM)	Aromatics (lumped on toluene)	18.6
CH_2O	Formaldehyde	16.6
C_2H_6	Ethane	12.1
HCOOH	Formic acid	10.9
C_3H_8	Propane	9.7
CHOCHO (GLY)	Glyoxal	8.5
$HOCH_2CHO$ (GLYAL)	Glycol-aldehyde	7.6
CH_3CH_2CHO (MGLY)	Methylglyoxal	5.1
C_2H_2	Acetylene	5.1
$CH_3CH_2COCH_3$ (MEK)	Methyl-ethyl-ketone (MEK)	3.3

CMIP6 - anthropogenic	C4H10	C2H4	CH3CHO	C2H2	MGLY	CH2O	CH3OH	HCOOH	CH3COOH	C2H6	CH3CH2OH	C3H8	C3H6	GLY	GLYAL	MEK	AROMATICS	ACETONE
VOC01-alcohols							X				X							
VOC02-ethane										X								
VOC03-propane												X						
VOC04-butanes	X																	
VOC05-pentanes	X																	
VOC06-hexanes-pl	X																	
VOC07-ethene		X																
VOC08-propene													X					
VOC09-ethyne				X														
VOC12-other-alke													X					
VOC13-benzene																	X	
VOC14-toluene																	X	
VOC15-xylene																	X	
VOC16-trimethylb																	X	
VOC17-other-arom																	X	
VOC21-methanal					X	X								X	X	X		
VOC22-other-alka			X															
VOC23-ketones																		X
VOC24-acids								X	X									

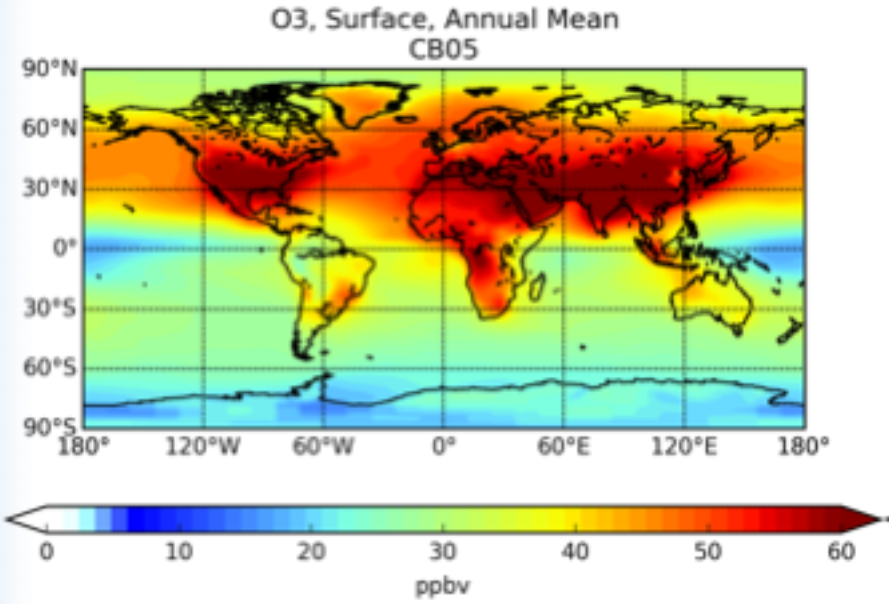
Coupling KPP with TM5-MP

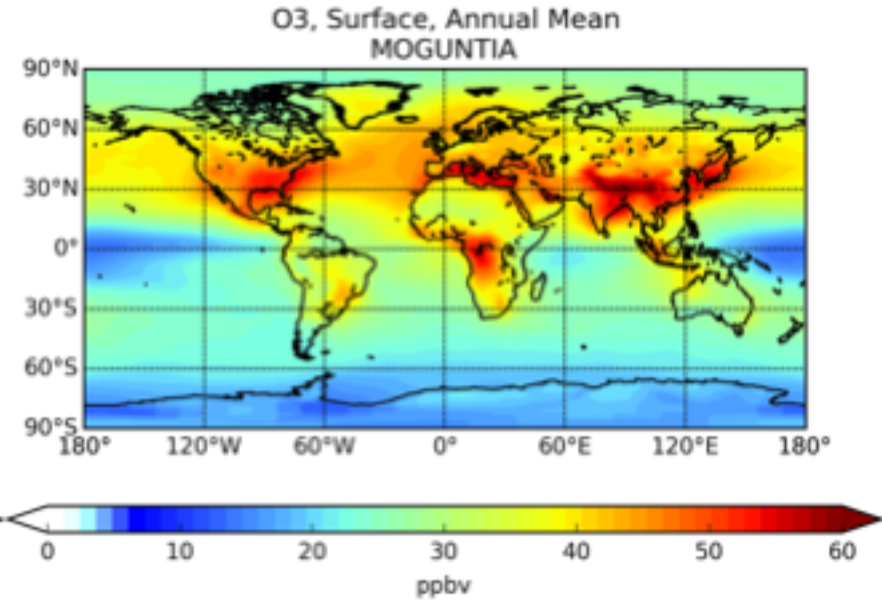
- The Kinetic PreProcessor (KPP) is a software that automatically generates code that solves a chemical scheme (defined by input files).
- KPP software tools are can be applied to any kinetic mechanism and provides a comprehensive suite of stiff numerical integrators (stiff solvers).
- The KPP framework allows to easily incorporate various solvers (e.g. **radau5**, **lsodes**, **runge_kutta**, **rosenbrock)** with the recommended solver to be the Rosenbrock Rodas3 (*Sandu and Sander, 2006*).
- KPP has been successfully integrated with major models (e.g., CMAQ, GEOS-Chem, STEM, ECHAM5/MESSy, WRF-Chem, C-IFS…) and provides a good combination of accuracy and efficiency.

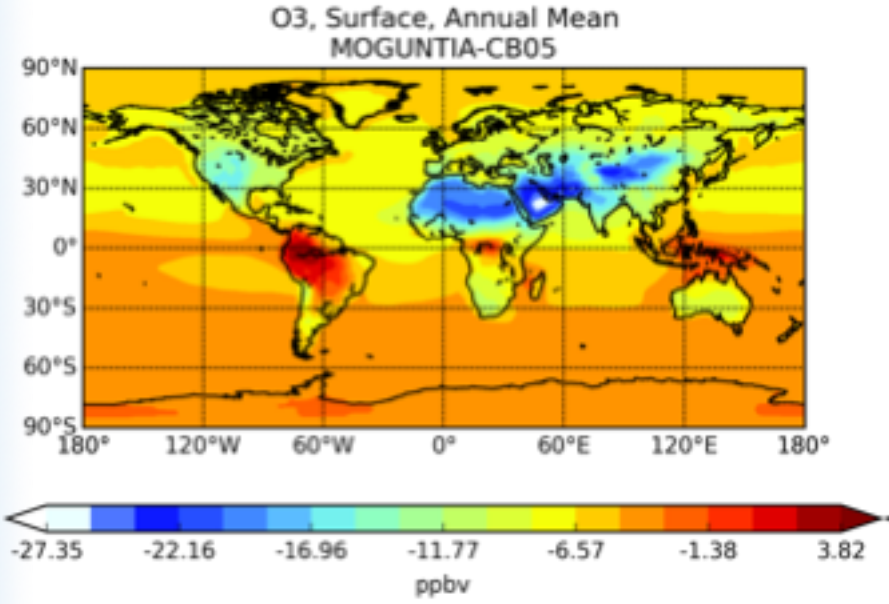
KPP-generated code…

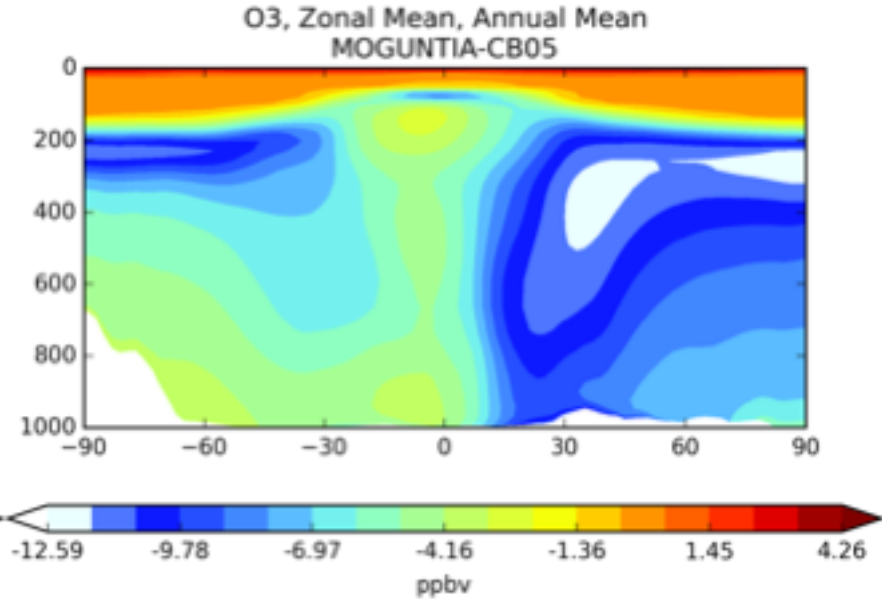
1) Write the gas- (and aqueous) phase mechanisms in KPP format
2) Create a new driver to interface the produced KPP files with the TM5 code
1) Preliminary tests show that the KPP-CB05 is ~14% slower than the standard EBI-CB05 solver for a glb600x400-tropo25 configuration (00:23:52 against 00:21:06 (hh:mm:ss) for JAN 2015; nx:4, ny: 6).

Ozone: CB05 vs MOGUNTIA

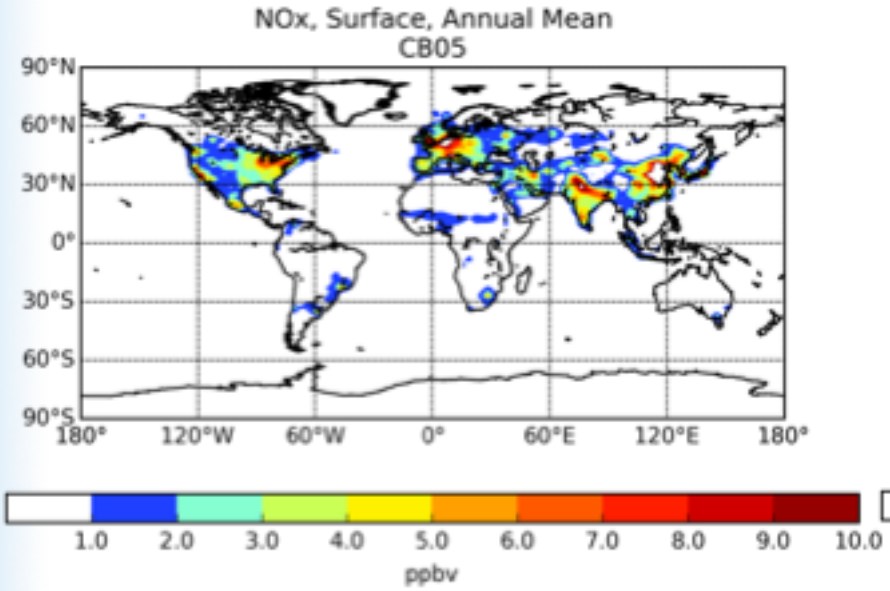


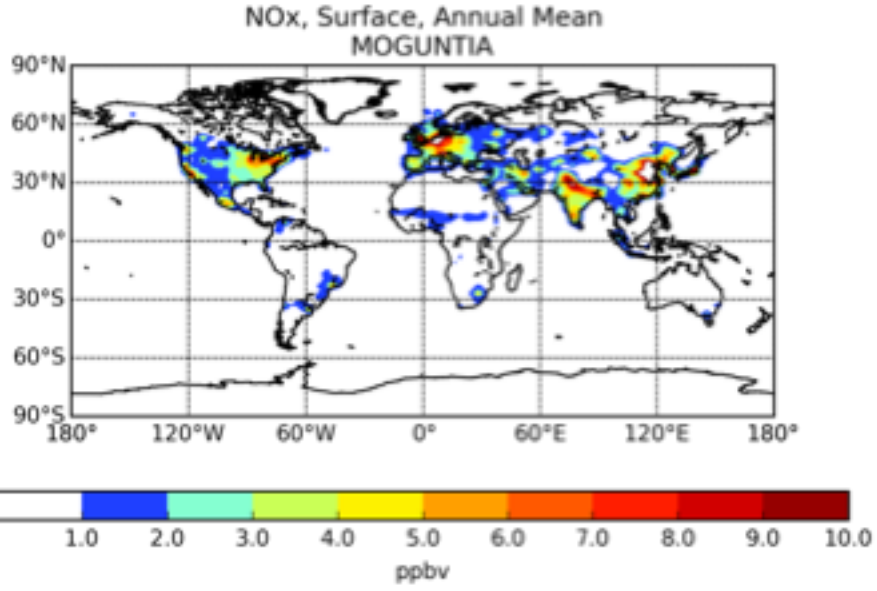


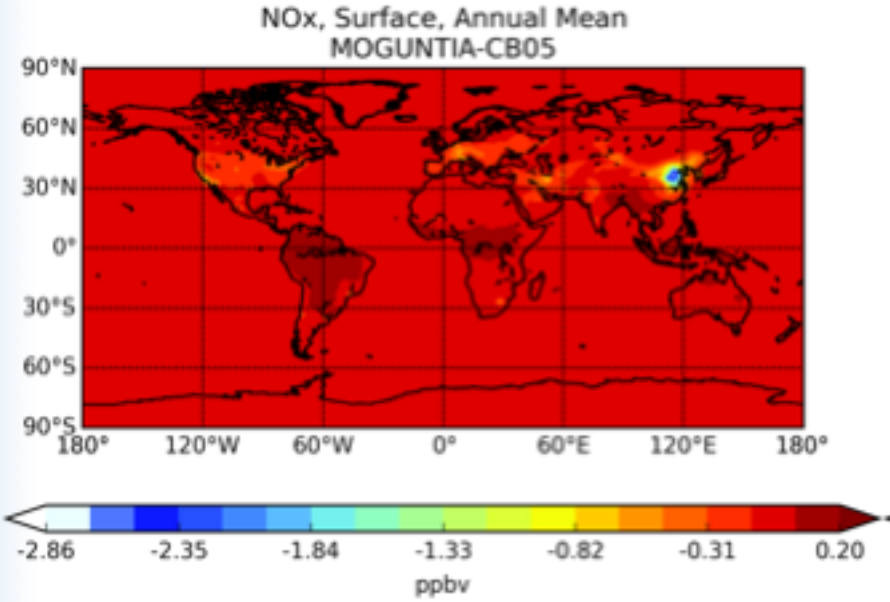


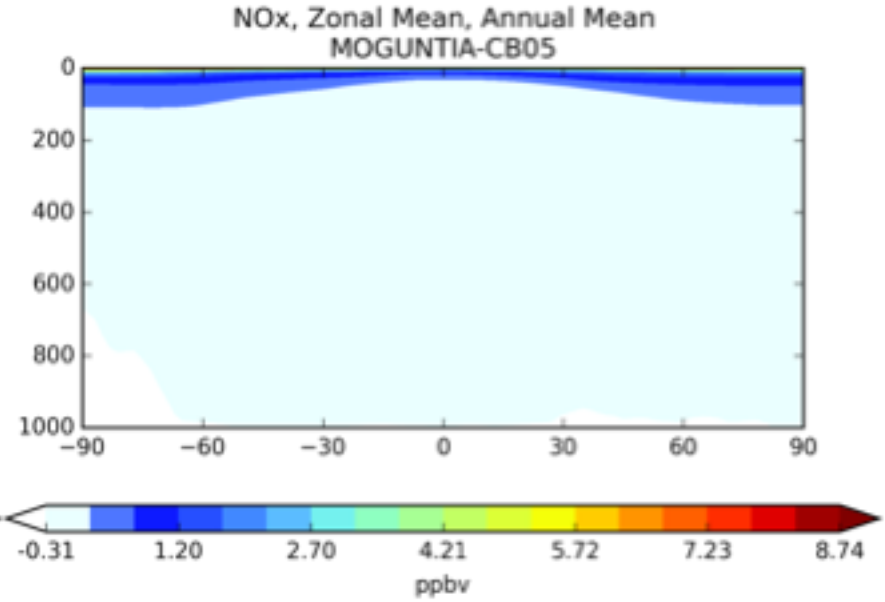


NOx: CB05 vs MOGUNTIA





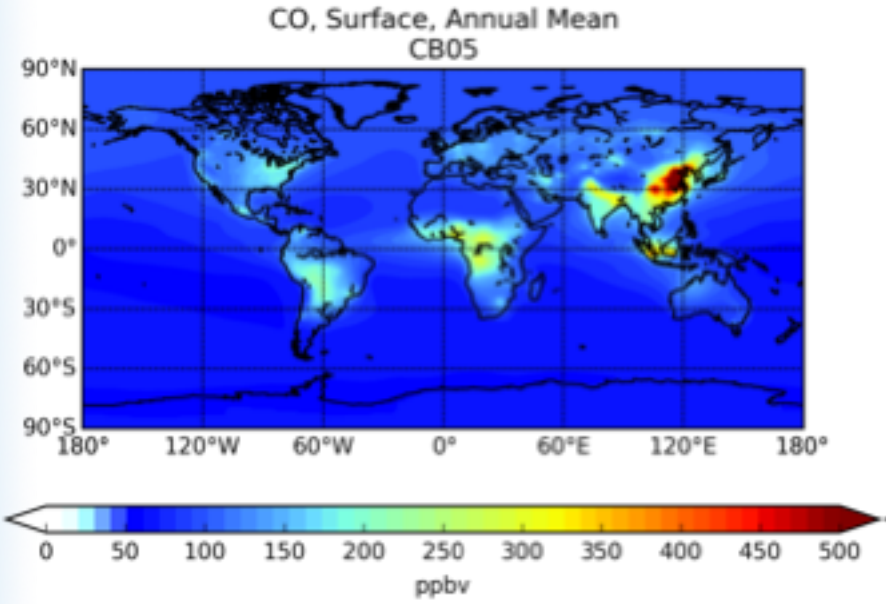


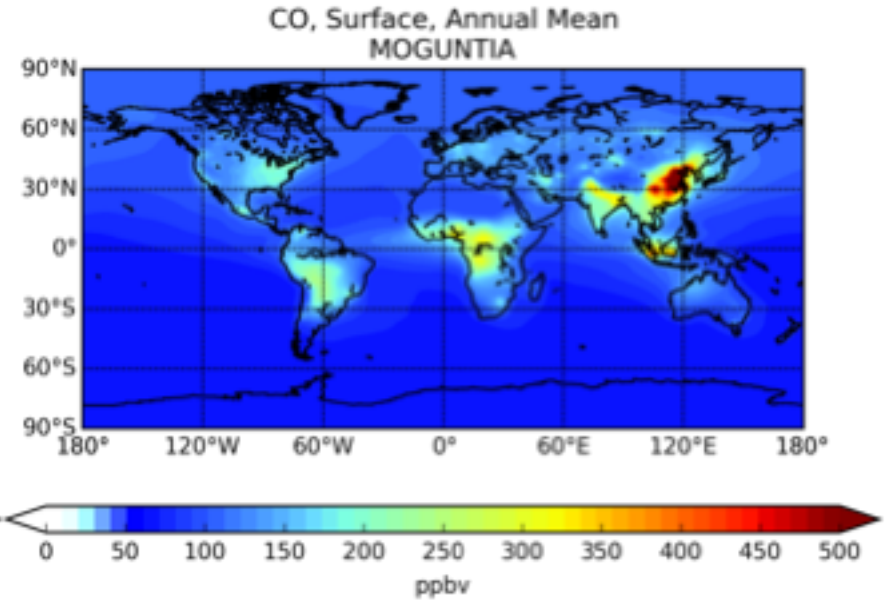


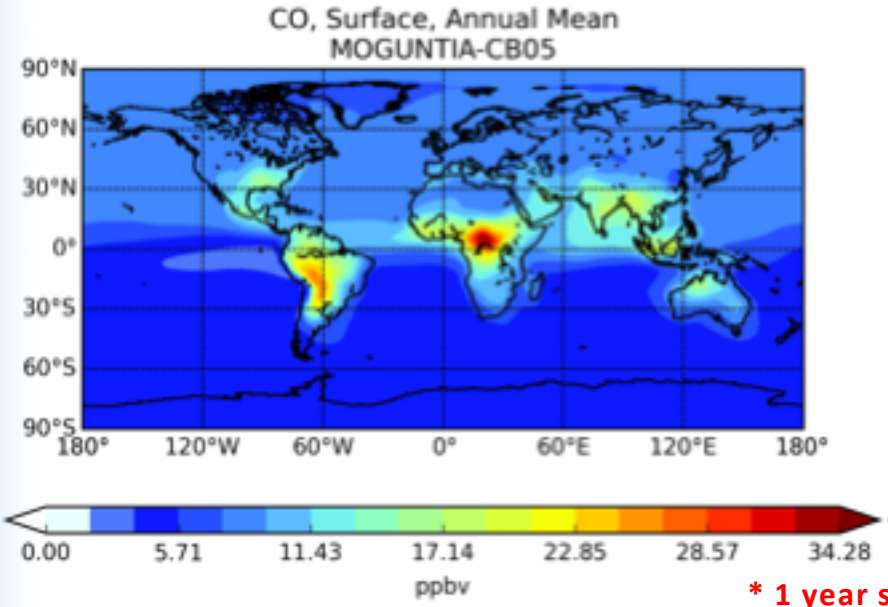
CO: CB05 vs MOGUNTIA

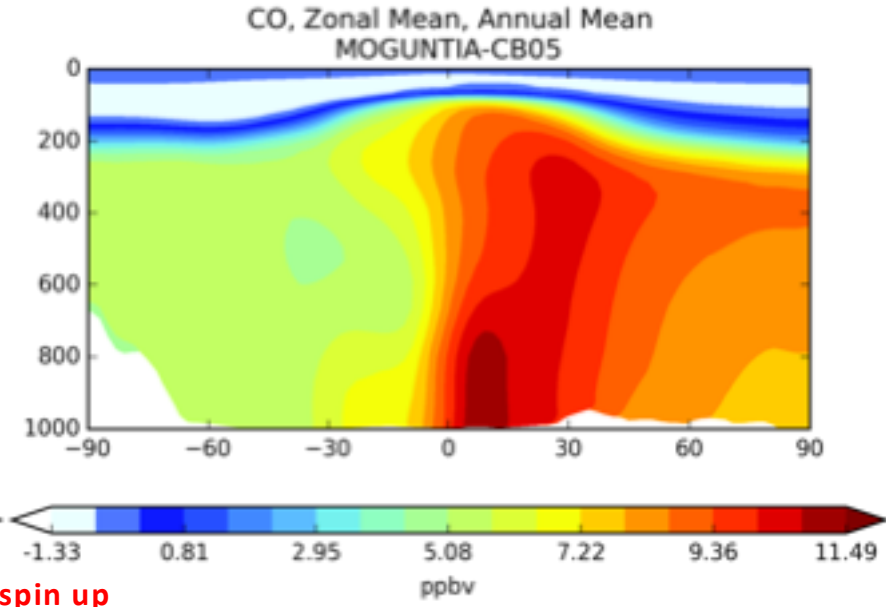
Global Lifetime*

64 days → 67 days



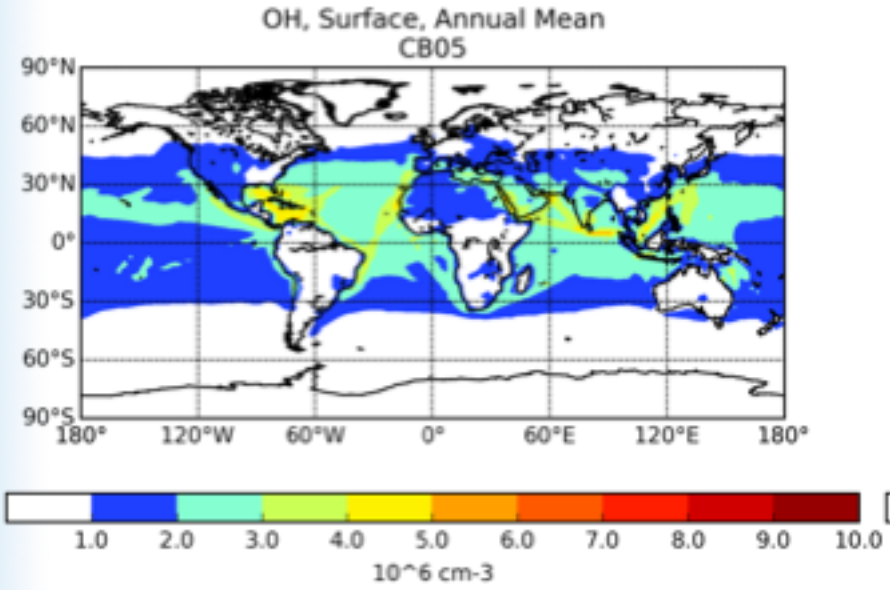


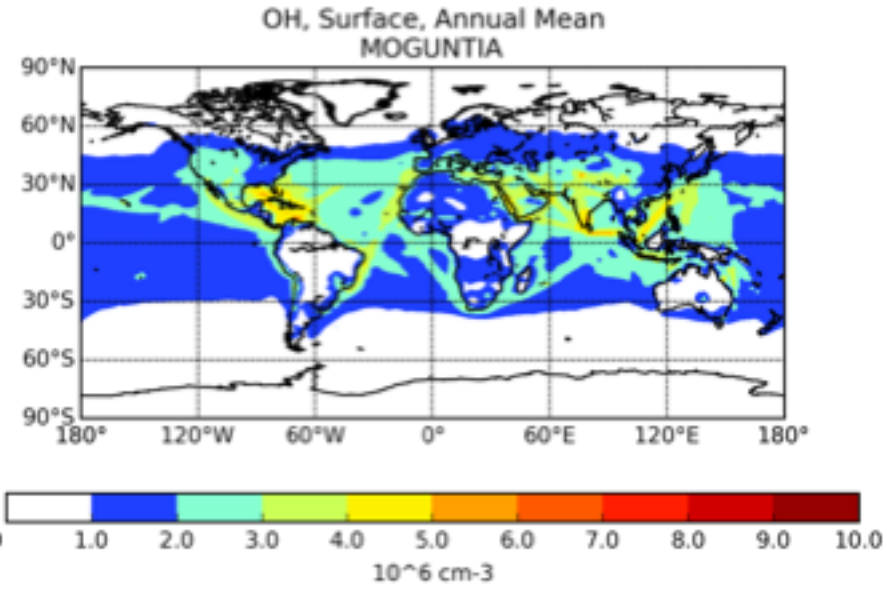


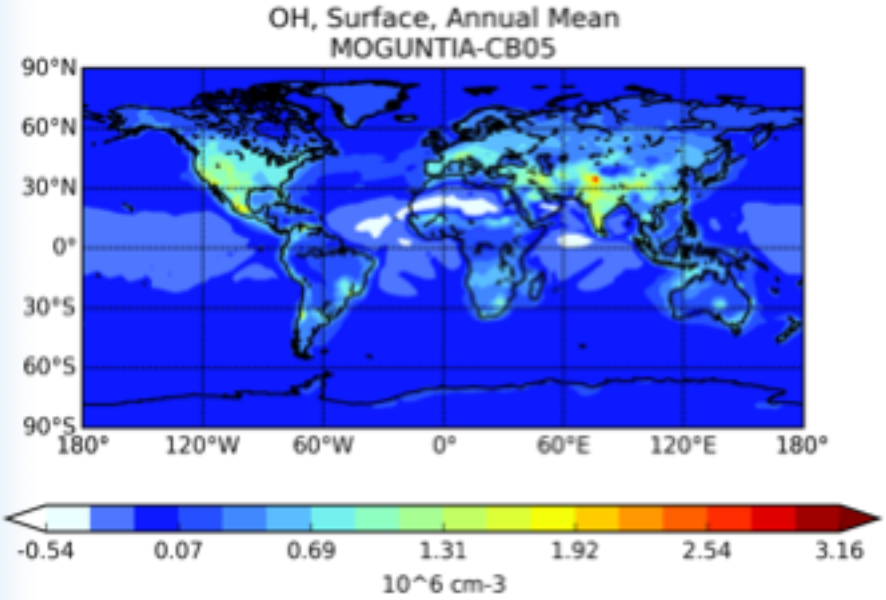


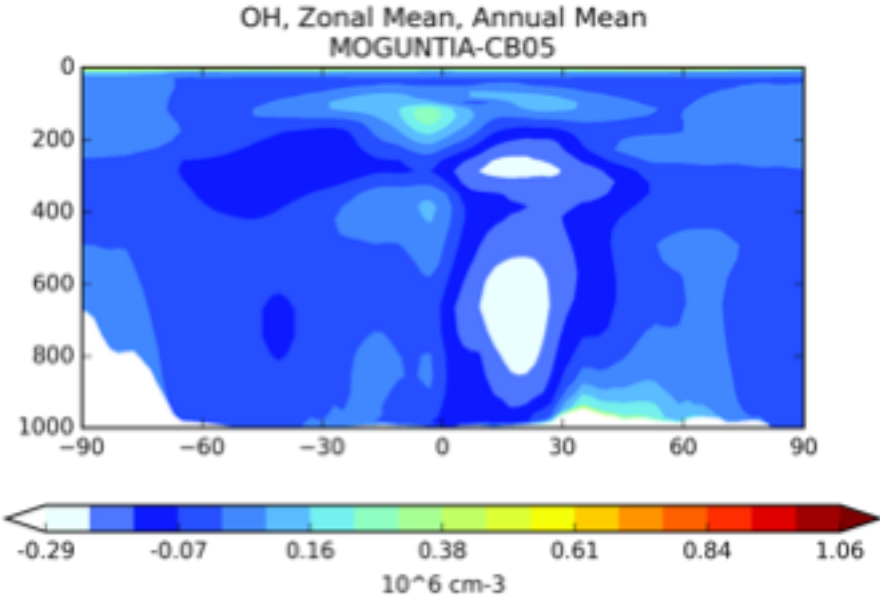
* 1 year spin up

OH: CB05 vs MOGUNTIA





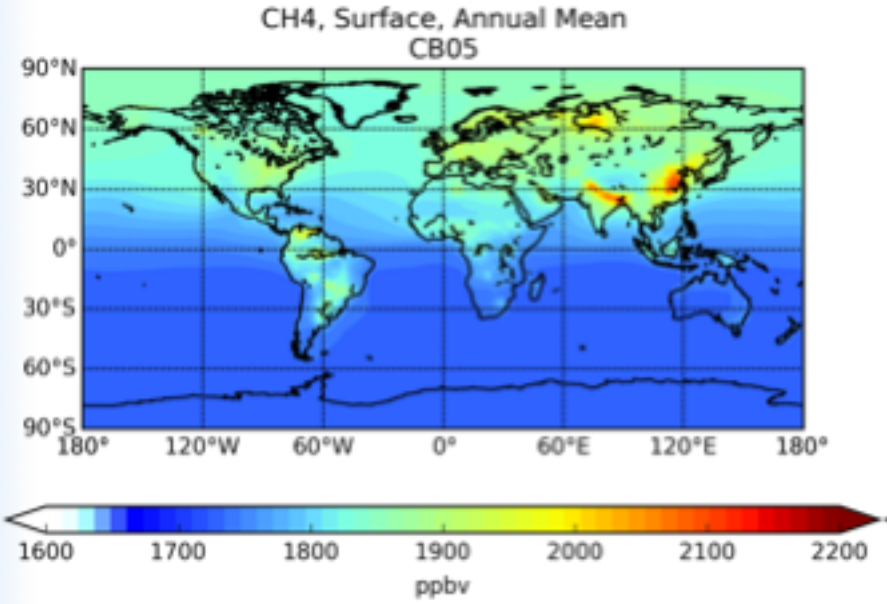


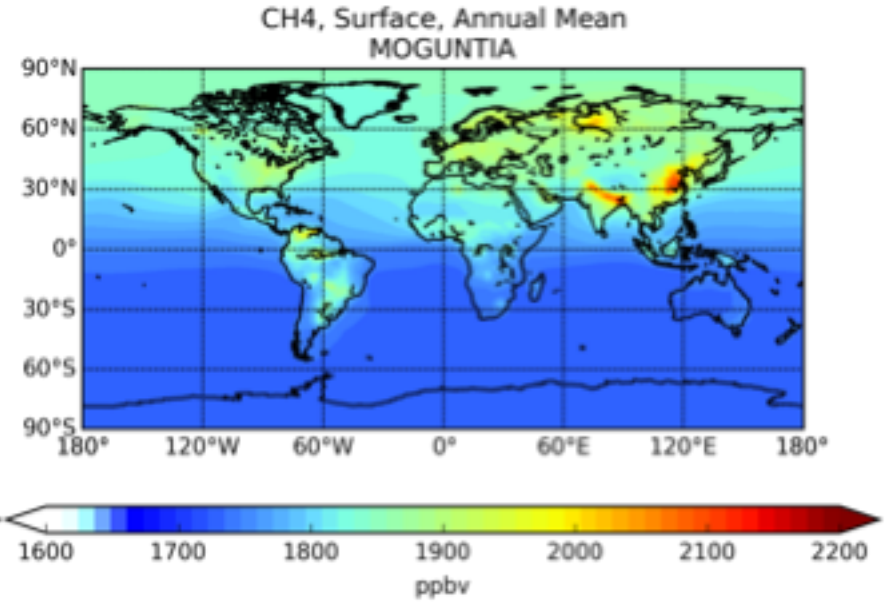


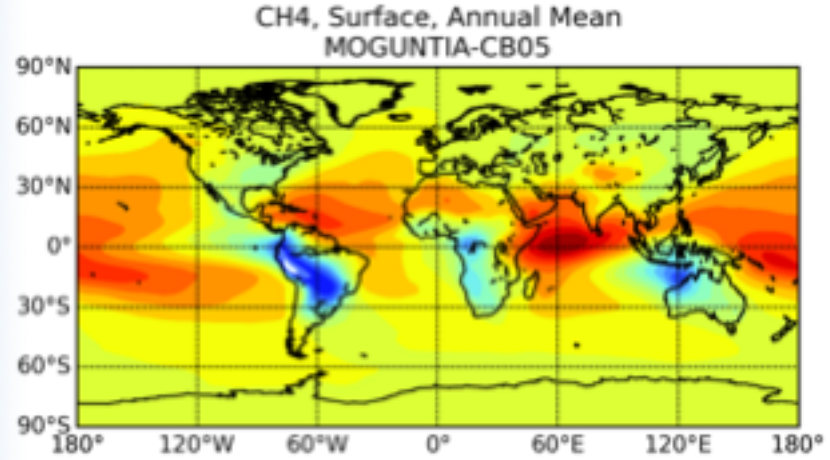
CH_4 : CB05 vs MOGUNTIA

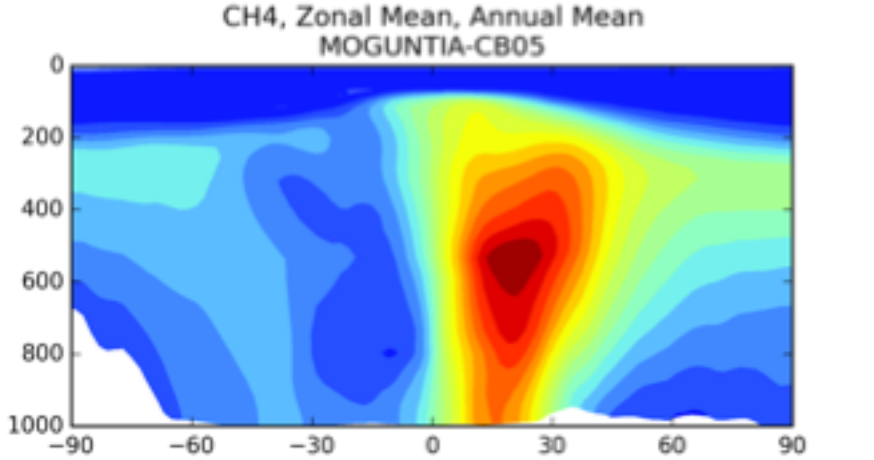
Global Lifetime*

8.1 years → 8.5 years



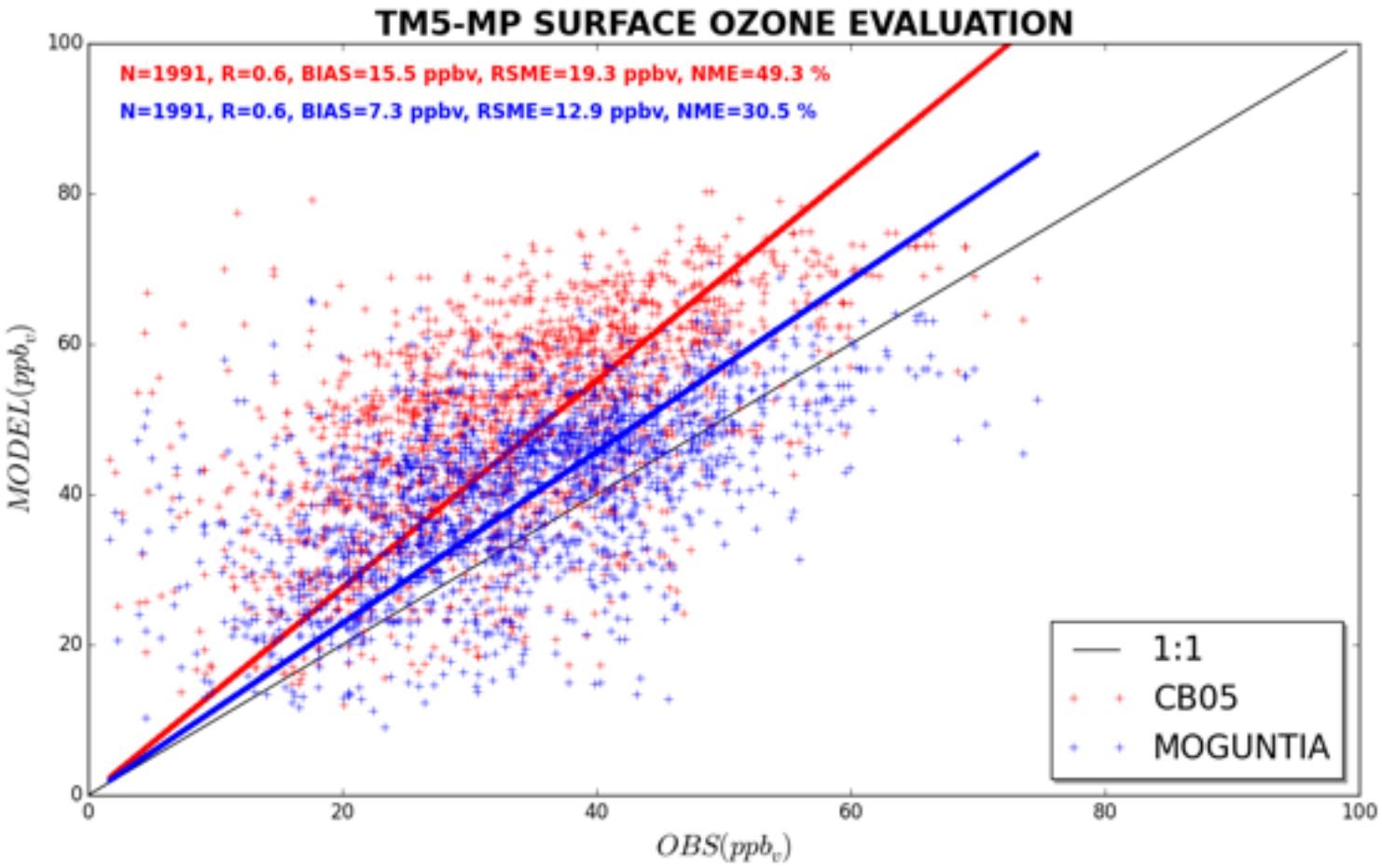






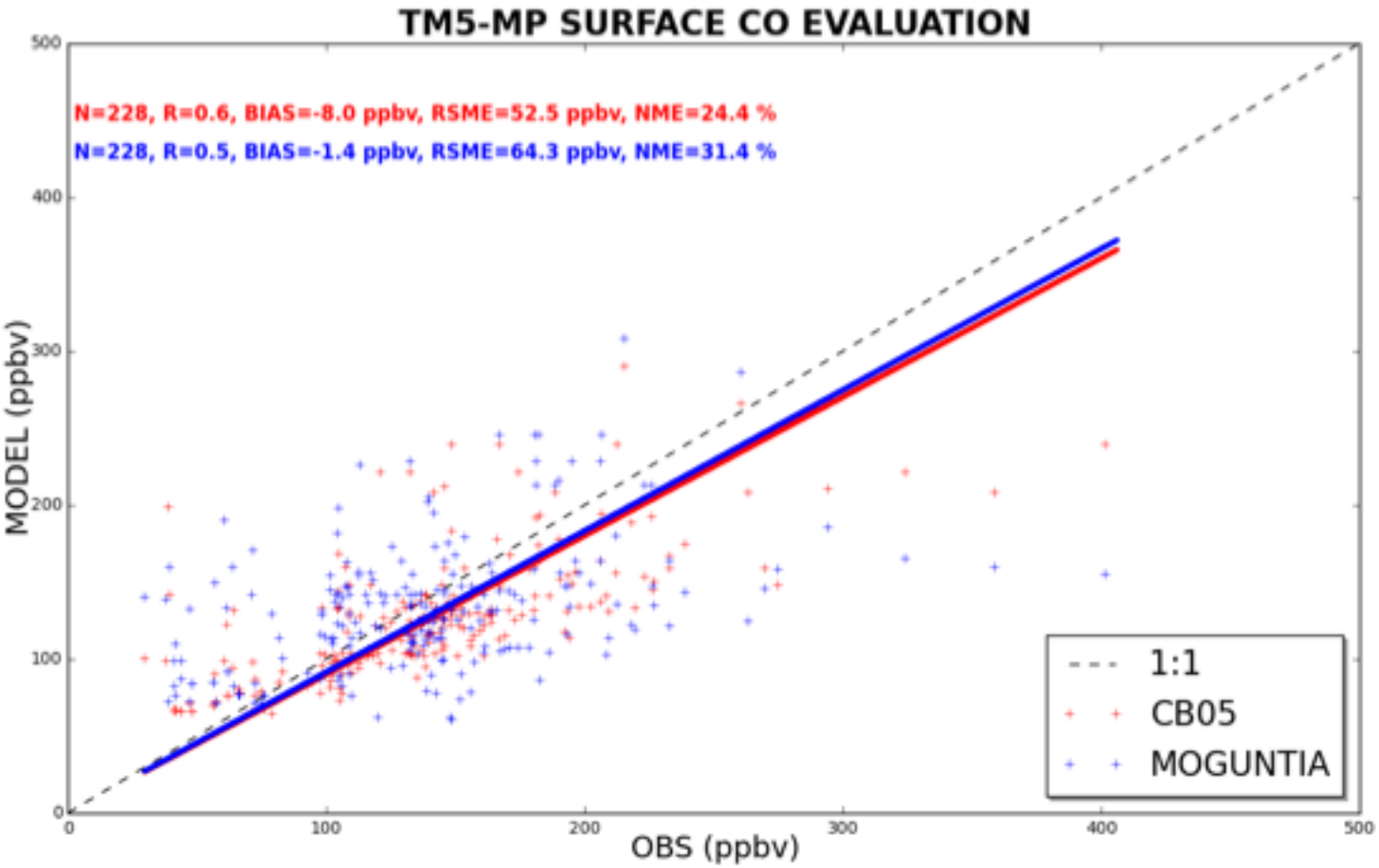
* 1 year spin up

Ozone Evaluation



O3 surface observations obtained from the World Data Centre for Greenhouse Gases (WDCGG; http://ds.data.jma.go.jp/gmd/wdcgg/introduction.html) and from the European Monitoring and Evaluation Programme (EMEP; http://www.emep.int).

CO Evaluation



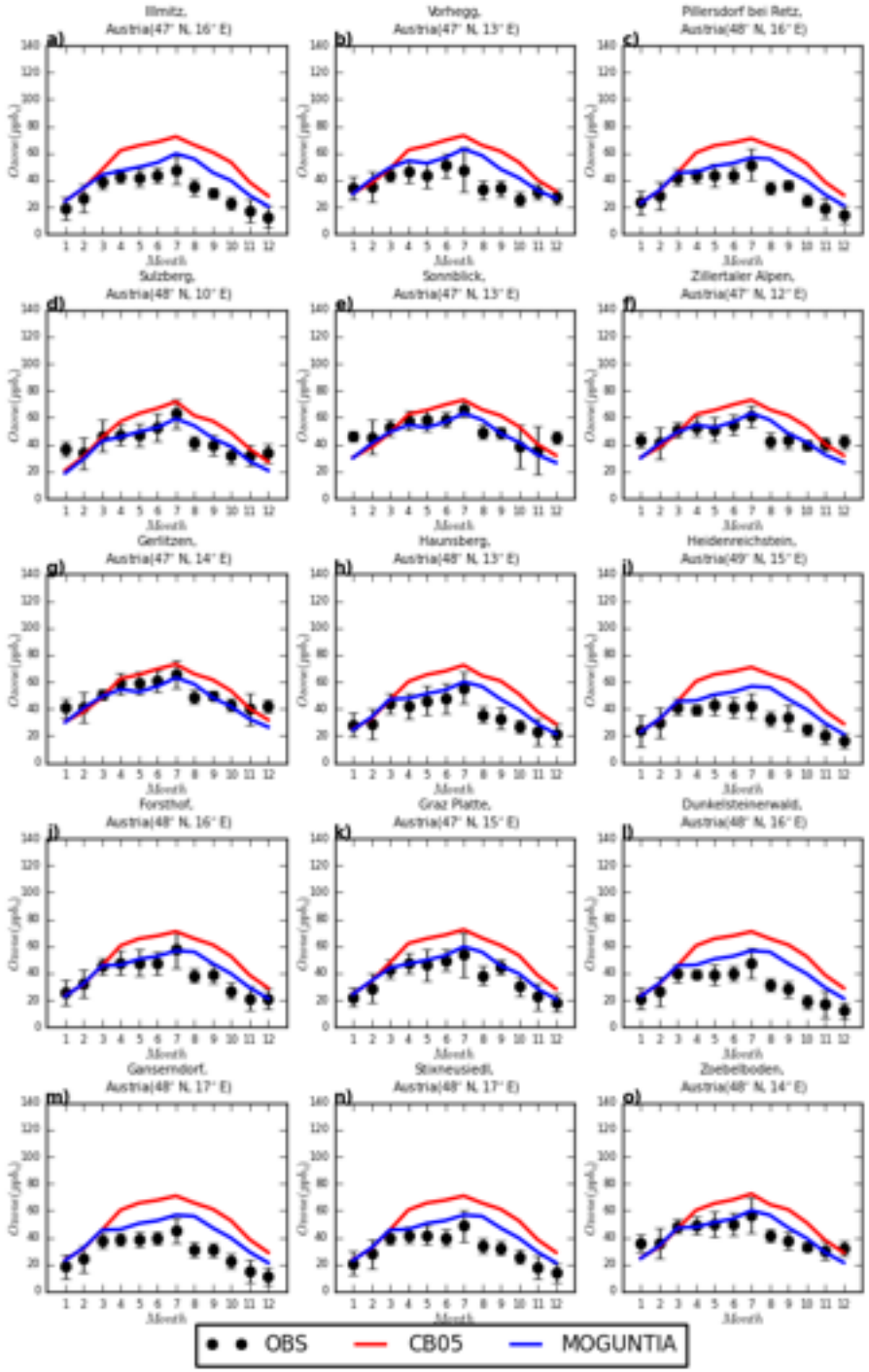
CO surface observations obtained from the World Data Centre for Greenhouse Gases (WDCGG; http://ds.data.jma.go.jp/gmd/wdcgg/introduction.html).

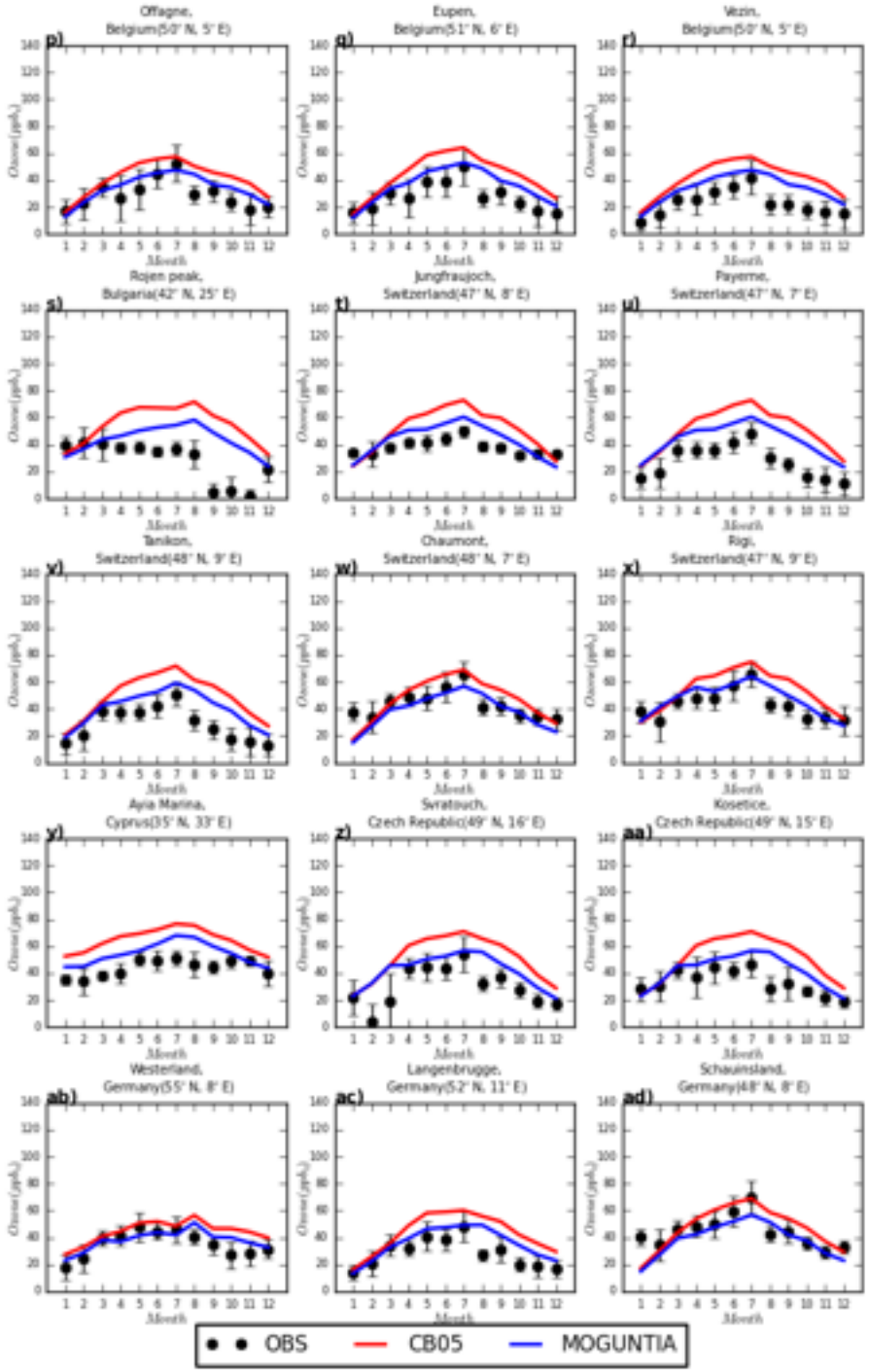
Summary

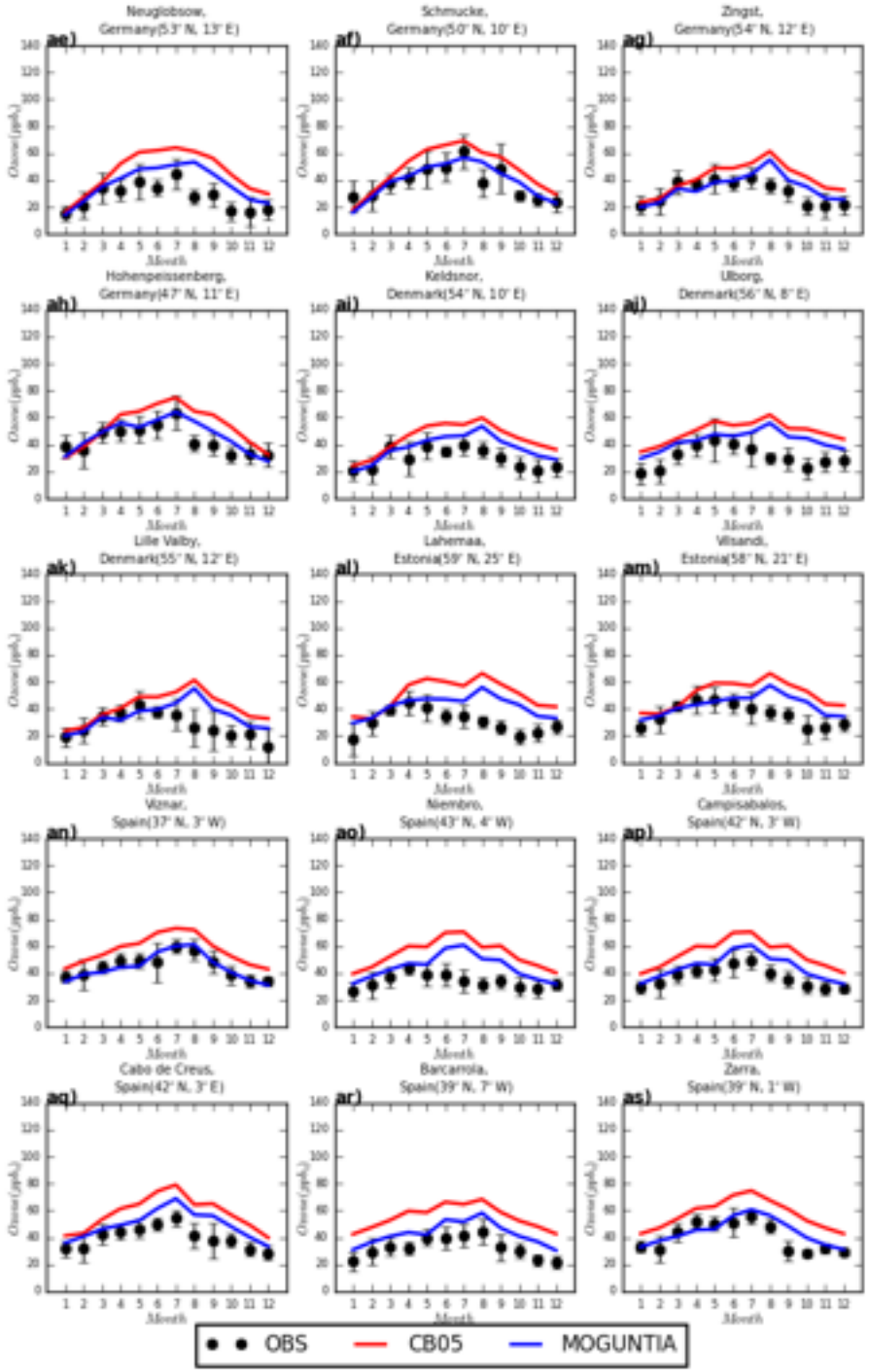
- TM5-MP is now also coupled with an explicit gas-phase chemical scheme (i.e., MOGUNTIA) - simulation year 2006 with one year (i.e., 2005) spin-up.
- MOGUNTIA (and CB05) chemical scheme is written in KPP.
- KPP-MOGUNTIA is ~28% slower than EBI-CB05 and ~12% than KPP-CB05, all for a glb600x400-tropo25 configuration.
- MOGUNTIA chemistry seems to improve the simulated O3 and CO validations with lower O3 and slighly higher CO global concentrations.
- Further developments:
  - TM5-MP is also coupled with a multiphase scheme in cloud droplets and wet aerosols
  - A „light“ AQCHEM version in implemented in EC-Earth but based on the CMB05 mechanism
  - A paper on the MOGUNTIA-TM5MP coupling is in preparation

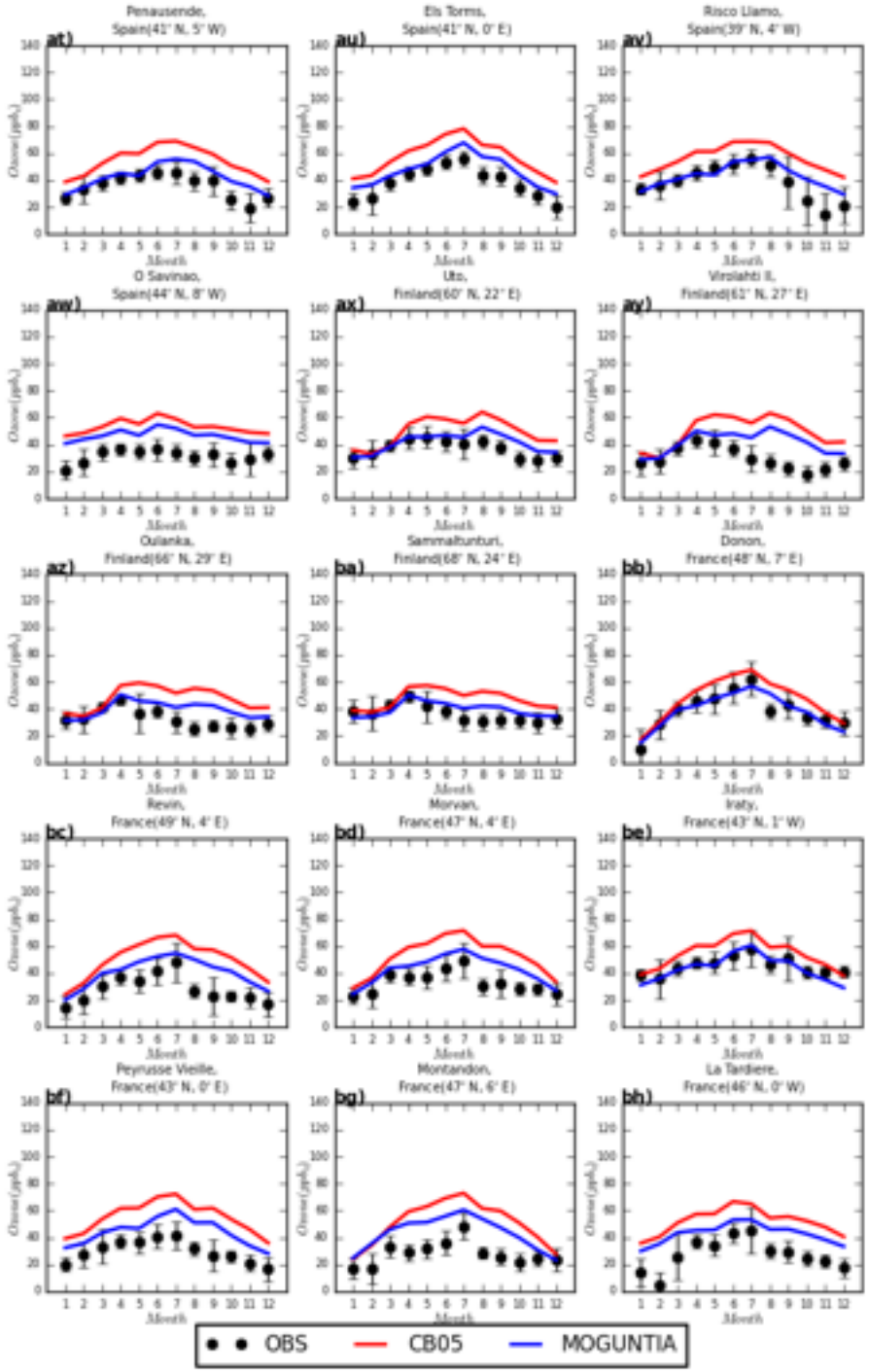
Appendix

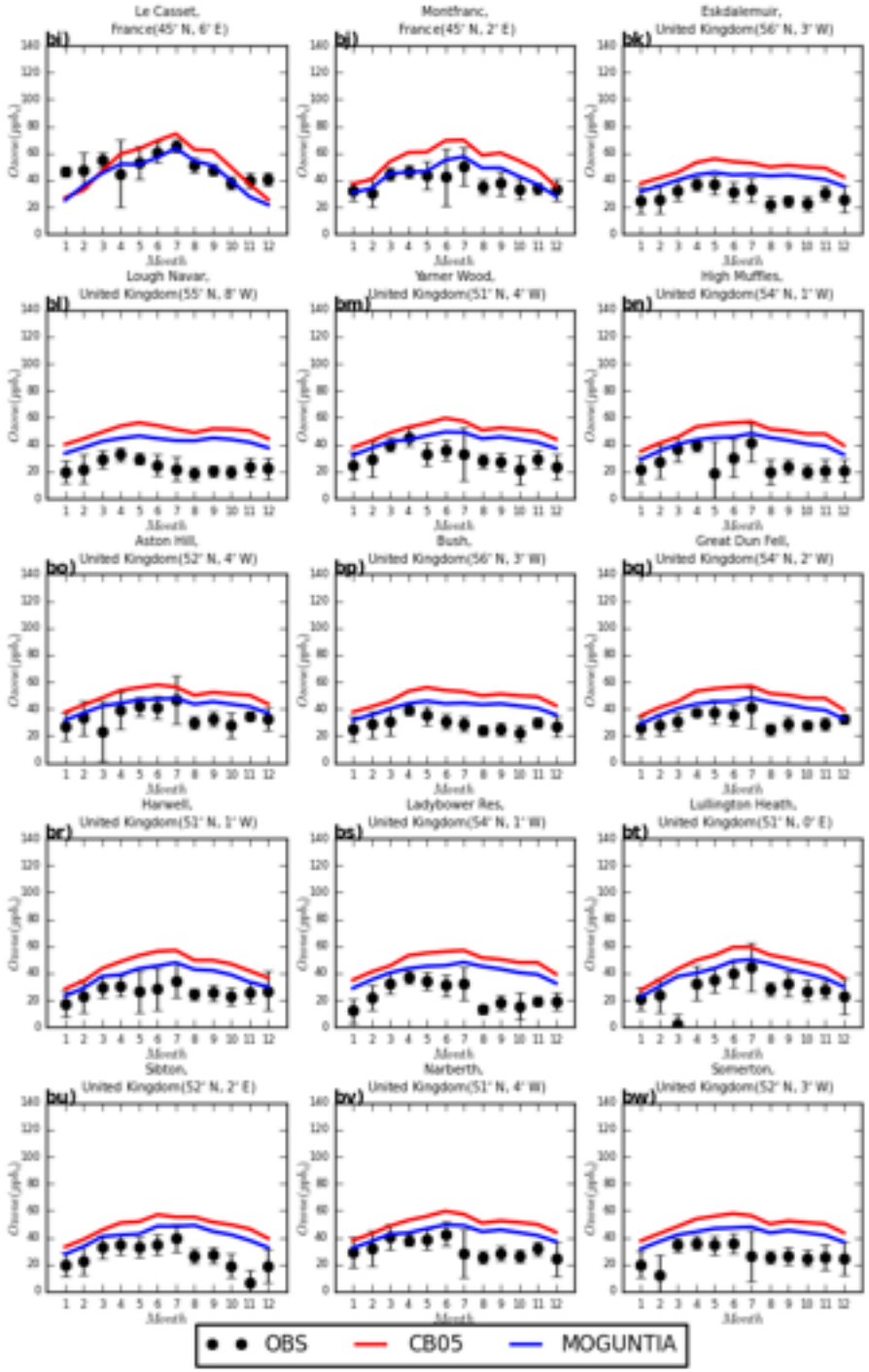
1. O_3

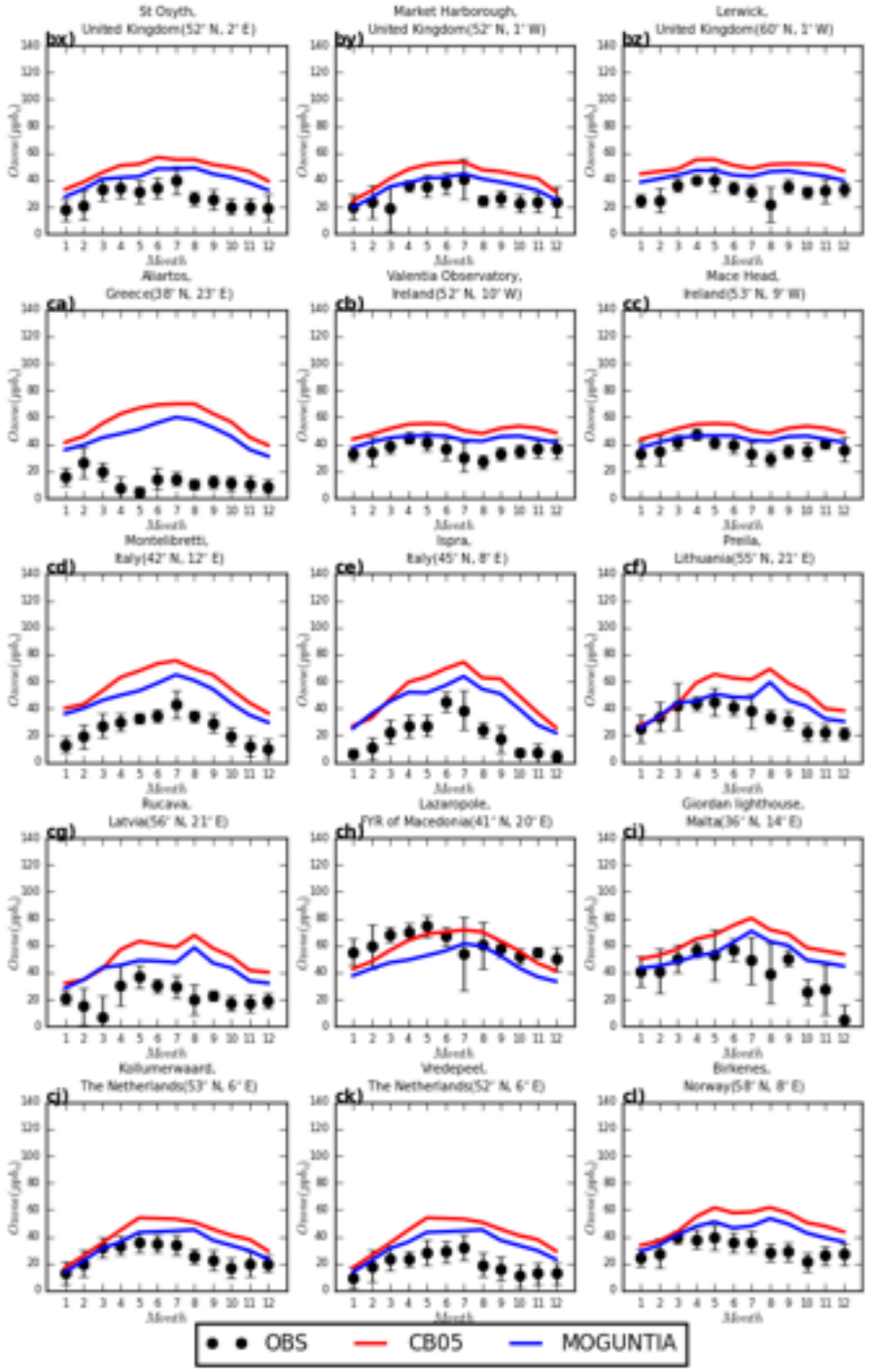

a) Illmitz, Austria(47° N, 16° E)
b) Vorhegg, Austria(47° N, 13° E)
c) Pillersdorf bei Retz, Austria(48° N, 16° E)
d) Sulzberg, Austria(48° N, 10° E)
e) Sonnblick, Austria(47° N, 13° E)
f) Zillertaler Alpen, Austria(47° N, 12° E)
g) Gerlitzen, Austria(47° N, 14° E)
h) Haunsberg, Austria(48° N, 13° E)
i) Heidenreichstein, Austria(49° N, 15° E)
j) Forsthof, Austria(48° N, 16° E)
k) Graz Platte, Austria(47° N, 15° E)
l) Dunkelsteinerwald, Austria(48° N, 16° E)
m) Ganserndorf, Austria(48° N, 17° E)
n) Stixneusiedl, Austria(48° N, 17° E)
o) Zwölfaxing, Austria(48° N, 14° E)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA


p) Offagne, Belgium(50° N, 5° E)
q) Eupen, Belgium(51° N, 6° E)
r) Vezin, Belgium(50° N, 5° E)
s) Rojen peak, Bulgaria(42° N, 25° E)
t) Jungfraujoch, Switzerland(47° N, 8° E)
u) Payerne, Switzerland(47° N, 7° E)
v) Tanikon, Switzerland(48° N, 9° E)
w) Chaumont, Switzerland(48° N, 7° E)
x) Rigi, Switzerland(47° N, 9° E)
y) Ayia Marina, Cyprus(35° N, 33° E)
z) Svratouch, Czech Republic(49° N, 16° E)
aa) Kosetice, Czech Republic(49° N, 15° E)
ab) Westerland, Germany(55° N, 8° E)
ac) Langenbrugge, Germany(52° N, 11° E)
ad) Schauinsland, Germany(48° N, 8° E)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA


ae)
Neuglobsow, Germany(53° N, 13° E)
af)
Schmucke, Germany(50° N, 10° E)
ag)
Zingst, Germany(54° N, 12° E)
ah)
Hohenpeissenberg, Germany(47° N, 11° E)
ai)
Keldsnor, Denmark(54° N, 10° E)
aj)
Ulborg, Denmark(56° N, 8° E)
ak)
Lille Valby, Denmark(55° N, 12° E)
al)
Lahemaa, Estonia(59° N, 25° E)
am)
Vilsandi, Estonia(58° N, 21° E)
an)
Viznar, Spain(37° N, 3° W)
ao)
Niembro, Spain(43° N, 4° W)
ap)
Campisabalos, Spain(42° N, 3° W)
aq)
Cabo de Creus, Spain(42° N, 3° E)
ar)
Barcarrola, Spain(39° N, 7° W)
as)
Zarra, Spain(39° N, 1° W)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA


Penausende, Spain(41° N, 5° W)
Els Torms, Spain(41° N, 0° E)
Risco Llamo, Spain(39° N, 4° W)
O Savinao, Spain(44° N, 8° W)
Uto, Finland(60° N, 22° E)
Virolahti II, Finland(61° N, 27° E)
Oulanka, Finland(66° N, 29° E)
Sammaltunturi, Finland(68° N, 24° E)
Donon, France(48° N, 7° E)
Revin, France(49° N, 4° E)
Morvan, France(47° N, 4° E)
Iraty, France(43° N, 1° W)
Peyrusse Vieille, France(43° N, 0° E)
Montandon, France(47° N, 6° E)
La Tardiere, France(46° N, 0° W)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA


Le Casset, France(45° N, 6° E)
bi)
Montfranc, France(45° N, 2° E)
bj)
Eskdalemuir, United Kingdom(56° N, 3° W)
bk)
Lough Navar, United Kingdom(55° N, 8° W)
bl)
Yarner Wood, United Kingdom(51° N, 4° W)
bm)
High Muffles, United Kingdom(54° N, 1° W)
bn)
Aston Hill, United Kingdom(52° N, 4° W)
bo)
Bush, United Kingdom(56° N, 3° W)
bp)
Great Dun Fell, United Kingdom(54° N, 2° W)
bq)
Harwell, United Kingdom(51° N, 1° W)
br)
Ladybower Res, United Kingdom(54° N, 1° W)
bs)
Lullington Heath, United Kingdom(51° N, 0° E)
bt)
Sibton, United Kingdom(52° N, 2° E)
bu)
Narberth, United Kingdom(51° N, 4° W)
bv)
Somerton, United Kingdom(52° N, 3° W)
bw)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA


St Osyth,
United Kingdom(52° N, 2° E)
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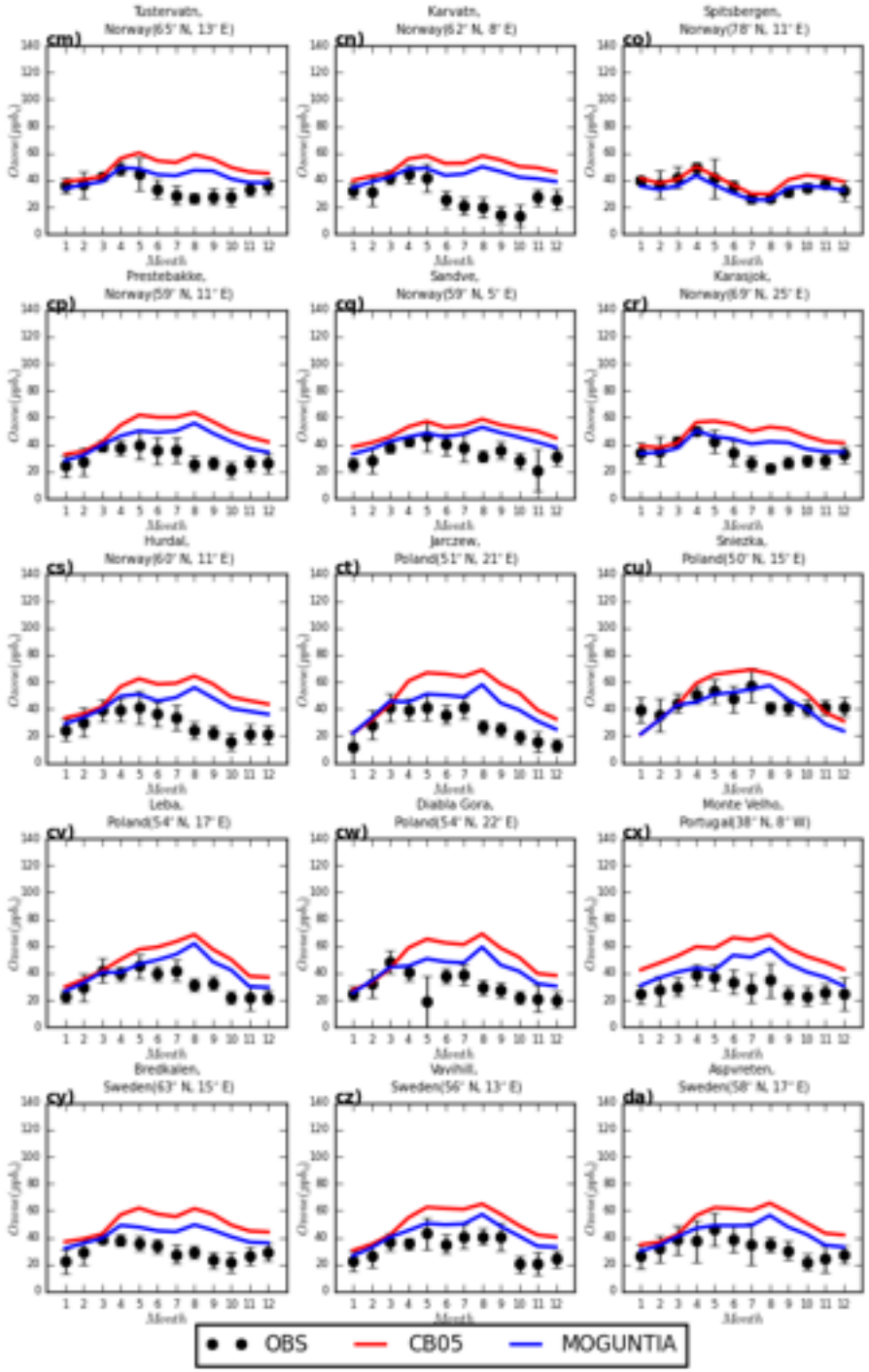
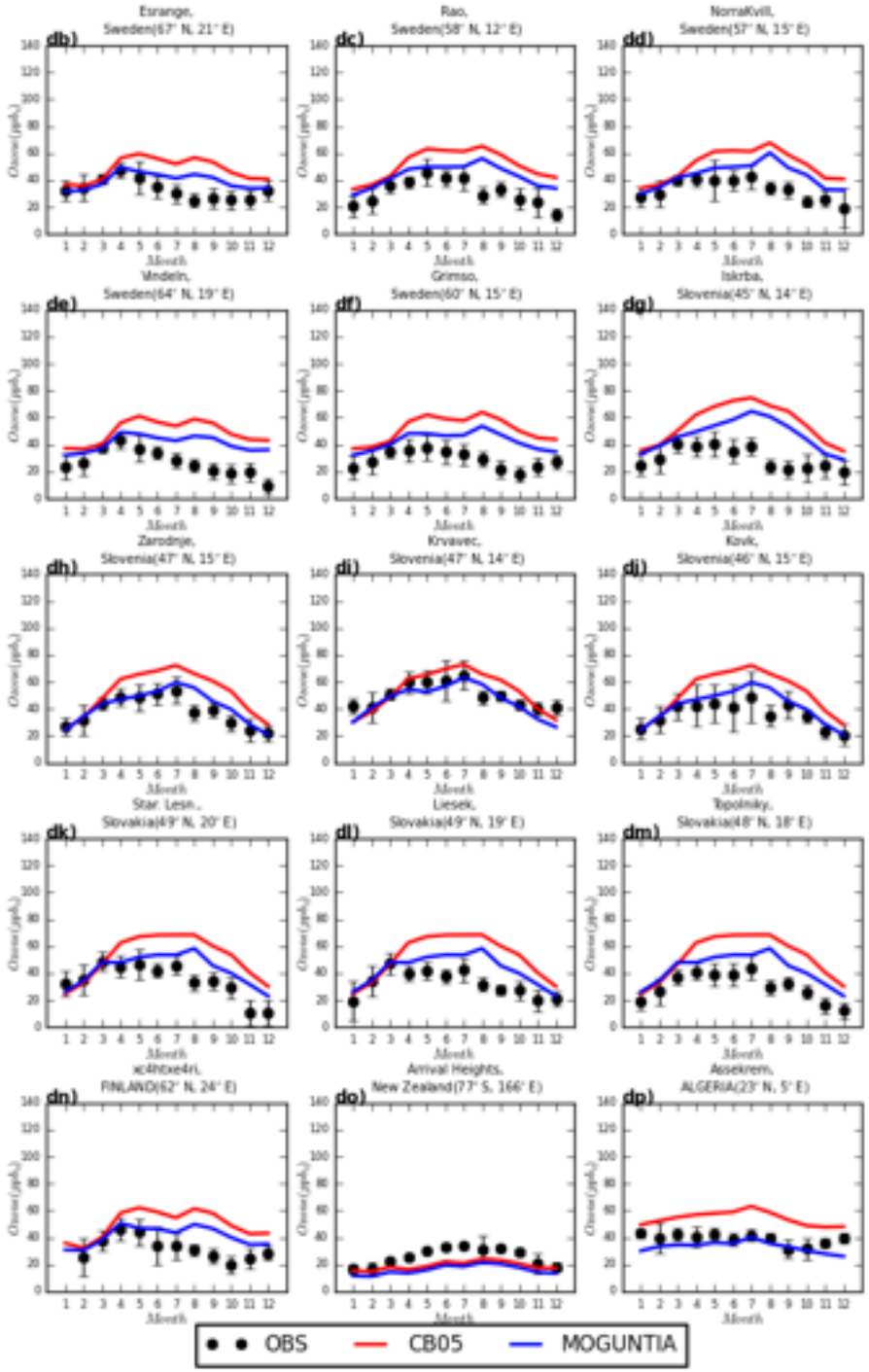
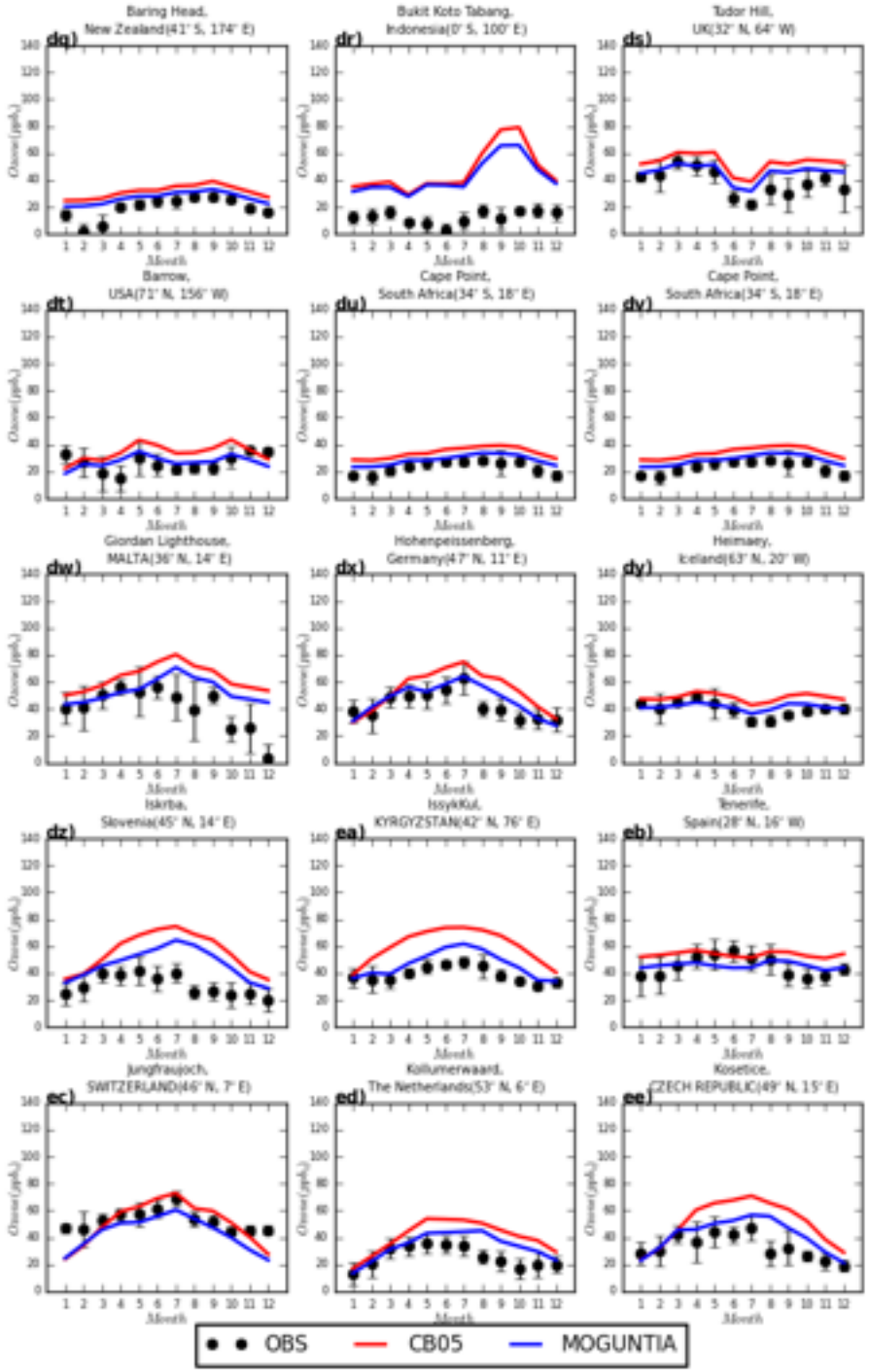
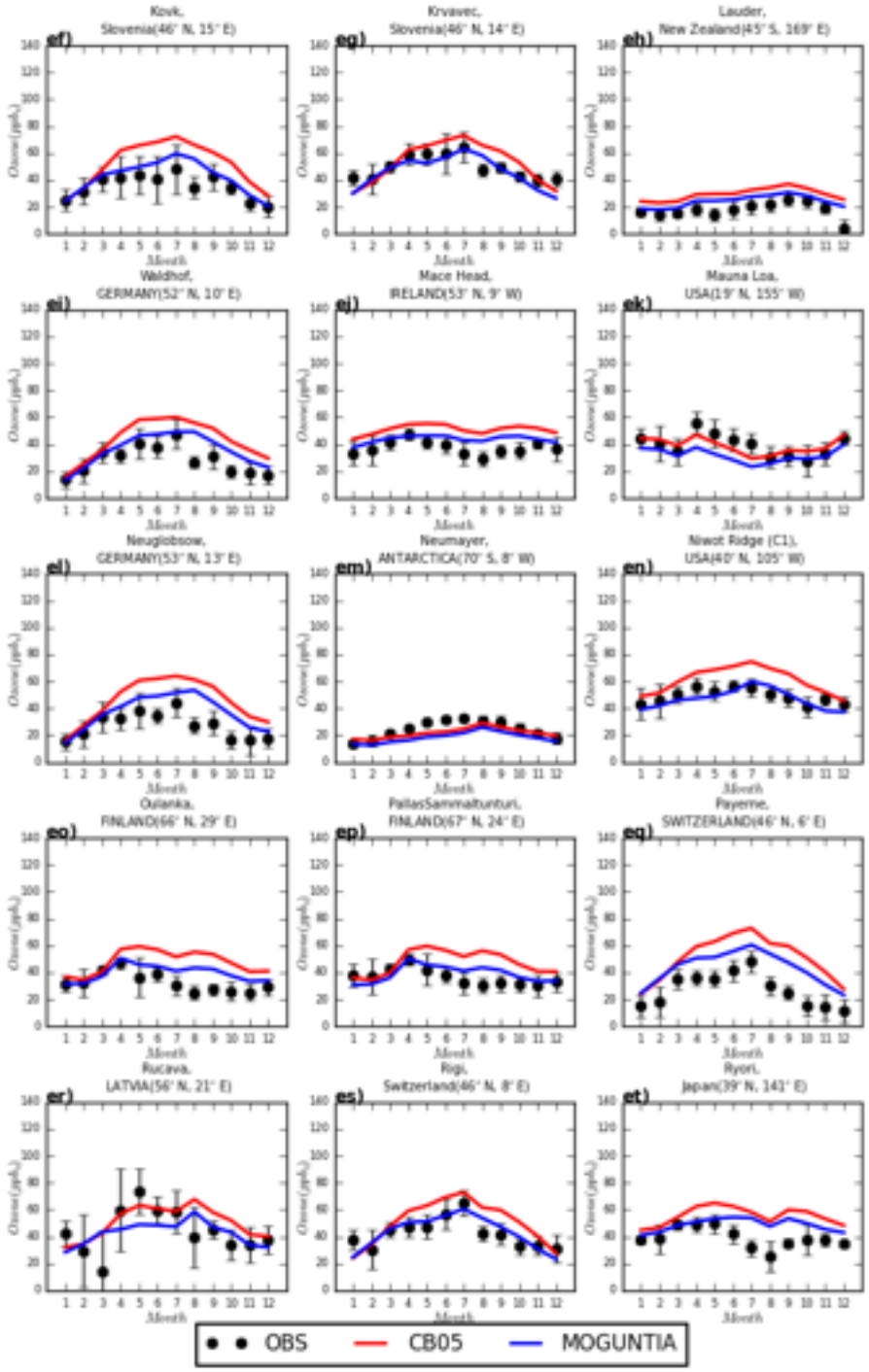
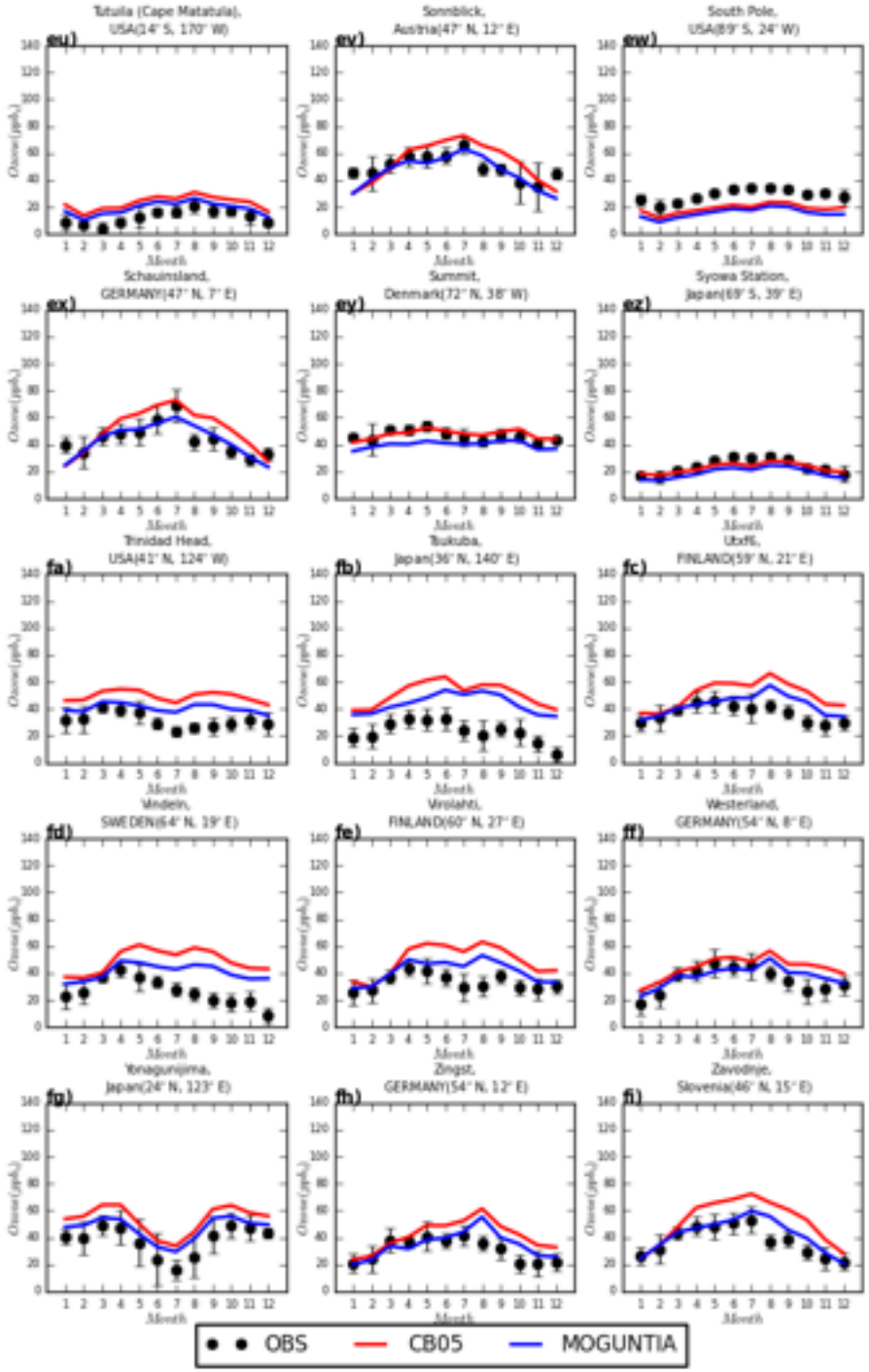
United Kingdom(52° N, 1° W)
by)
Lerwick,
United Kingdom(60° N, 1° W)
bz)
Aliartos,
Greece(38° N, 23° E)
ca)
Valentia Observatory,
Ireland(52° N, 10° W)
cb)
Mace Head,
Ireland(53° N, 9° W)
cc)
Montelibretti,
Italy(42° N, 12° E)
cd)
Ispra,
Italy(45° N, 8° E)
ce)
Preila,
Lithuania(55° N, 21° E)
cf)
Rucava,
Latvia(56° N, 21° E)
cg)
Lazaropole,
FYR of Macedonia(41° N, 20° E)
ch)
Giordan lighthouse,
Malta(36° N, 14° E)
ci)
Kollumerwaard,
The Netherlands(53° N, 6° E)
cj)
Vredepeel,
The Netherlands(52° N, 6° E)
ck)
Birkenes,
Norway(58° N, 8° E)
cl)
Ozone (ppb)
Month
OBS
CB05
MOGUNTIA


Tustervatn, Norway(65° N, 13° E)
cm)
Karvatn, Norway(62° N, 8° E)
cn)
Spitsbergen, Norway(78° N, 11° E)
co)
Prestebakke, Norway(59° N, 11° E)
cp)
Sandve, Norway(59° N, 5° E)
cq)
Karasjok, Norway(69° N, 25° E)
cr)
Hurdal, Norway(60° N, 11° E)
cs)
Jarczew, Poland(51° N, 21° E)
ct)
Sniezka, Poland(50° N, 15° E)
cu)
Leba, Poland(54° N, 17° E)
cv)
Diabla Gora, Poland(54° N, 22° E)
cw)
Monte Velho, Portugal(38° N, 8° W)
cx)
Bredkalen, Sweden(63° N, 15° E)
cy)
Vavihill, Sweden(56° N, 13° E)
cz)
Aspvreten, Sweden(58° N, 17° E)
da)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA

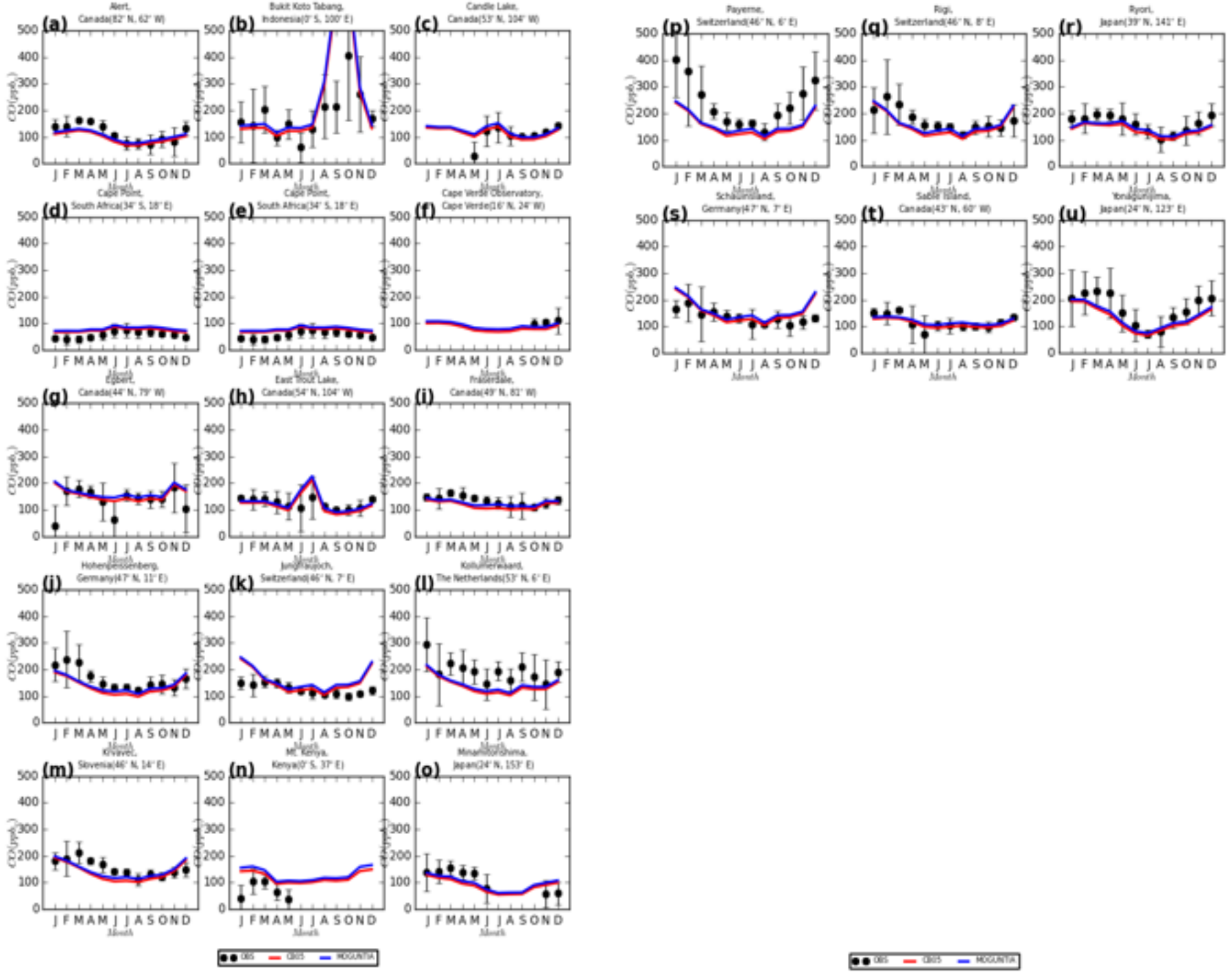

Esrange,
Sweden(67° N, 21° E)
db)
Rao,
Sweden(58° N, 12° E)
dc)
Norrakvill,
Sweden(57° N, 15° E)
dd)
Vindeln,
Sweden(64° N, 19° E)
de)
Grimso,
Sweden(60° N, 15° E)
df)
Iskrba,
Slovenia(45° N, 14° E)
dg)
Zarodnje,
Slovenia(47° N, 15° E)
dh)
Krvavec,
Slovenia(47° N, 14° E)
di)
Kovk,
Slovenia(46° N, 15° E)
dj)
Star. Lesn.,
Slovakia(49° N, 20° E)
dk)
Liesek,
Slovakia(49° N, 19° E)
dl)
Topolniky,
Slovakia(48° N, 18° E)
dm)
xc4htxe4ri,
FINLAND(62° N, 24° E)
dn)
Arrival Heights,
New Zealand(77° S, 166° E)
do)
Assekrem,
ALGERIA(23° N, 5° E)
dp)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA


Baring Head,
New Zealand(41° S, 174° E)
(dq)
Bukit Koto Tabang,
Indonesia(0° S, 100° E)
(dr)
Tudor Hill,
UK(32° N, 64° W)
(ds)
Barrow,
USA(71° N, 156° W)
(dt)
Cape Point,
South Africa(34° S, 18° E)
(du)
Cape Point,
South Africa(34° S, 18° E)
(dv)
Giordan Lighthouse,
MALTA(36° N, 14° E)
(dw)
Hohenpeissenberg,
Germany(47° N, 11° E)
(dx)
Heimaey,
Iceland(63° N, 20° W)
(dy)
Iskrba,
Slovenia(45° N, 14° E)
(dz)
IssykKul,
KYRGYZSTAN(42° N, 76° E)
(ea)
Teverite,
Spain(28° N, 16° W)
(eb)
Jungfraujoch,
SWITZERLAND(46° N, 7° E)
(ec)
Kollumerwaard,
The Netherlands(53° N, 6° E)
(ed)
Kosetice,
CZECH REPUBLIC(49° N, 15° E)
(ee)
Ozone (ppbv)
Month
OBS
CB05
MOGUNTIA

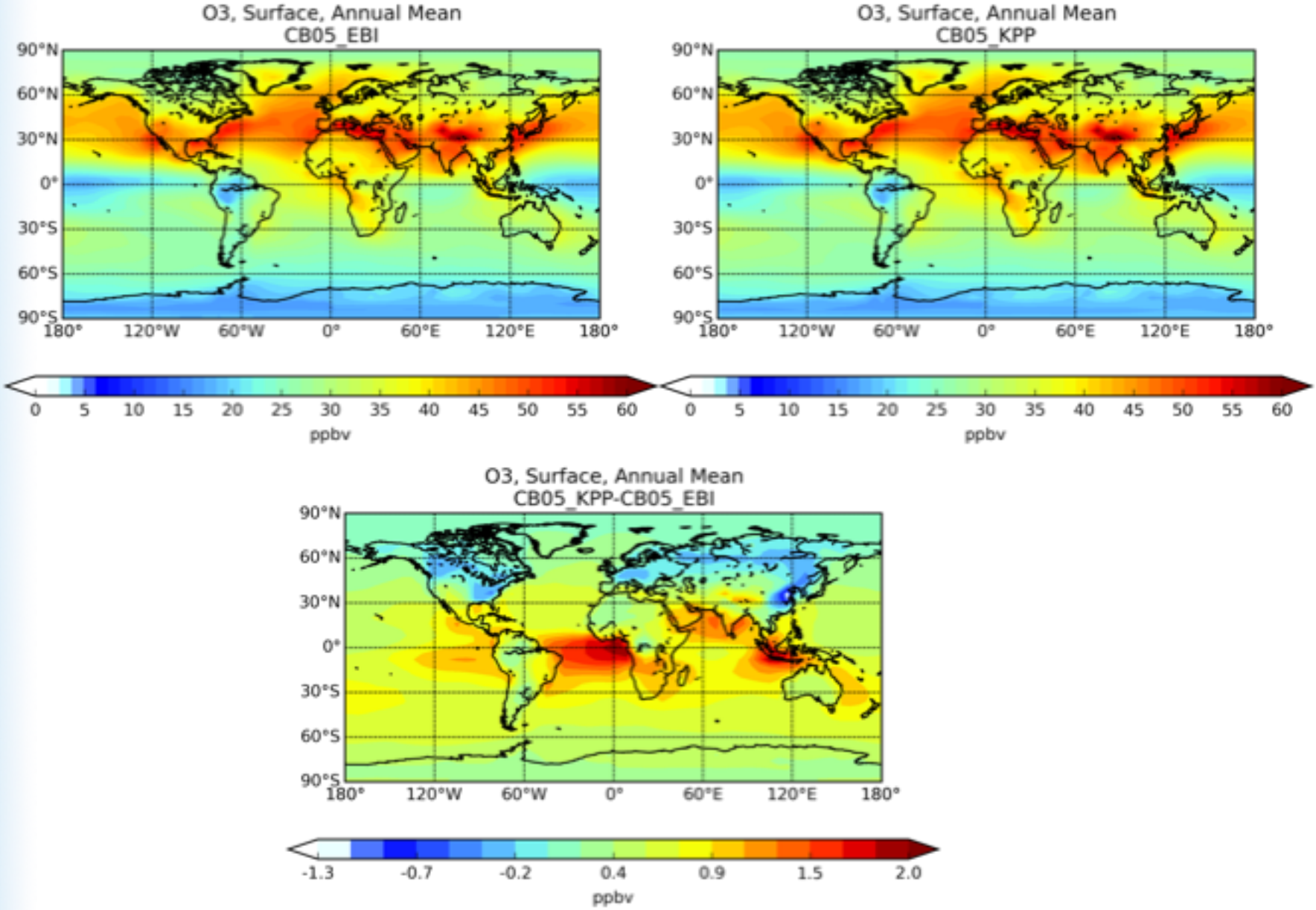

Kovk,
Slovenia(46° N, 15° E)
ef)
Krvavec,
Slovenia(46° N, 14° E)
eg)
Lauder,
New Zealand(45° S, 169° E)
eh)
Waldhof,
GERMANY(52° N, 10° E)
ei)
Mace Head,
IRELAND(53° N, 9° W)
ej)
Mauna Loa,
USA(19° N, 155° W)
ek)
Neuglobsow,
GERMANY(53° N, 13° E)
el)
Neumayer,
ANTARCTICA(70° S, 8° W)
em)
Niwot Ridge (C1),
USA(40° N, 105° W)
en)
Oulanka,
FINLAND(66° N, 29° E)
eo)
PallasSammaltunturi,
FINLAND(67° N, 24° E)
ep)
Payerne,
SWITZERLAND(46° N, 6° E)
eq)
Rucava,
LATVIA(56° N, 21° E)
er)
Rigi,
Switzerland(46° N, 8° E)
es)
Ryori,
Japan(39° N, 141° E)
et)
Month
OBS
CB05
MOGUNTIA


Tutuila (Cape Matatula), USA(14° S, 170° W)
Sonnblick, Austria(47° N, 12° E)
South Pole, USA(89° S, 24° W)
Schauinsland, GERMANY(47° N, 7° E)
Summit, Denmark(72° N, 38° W)
Syowa Station, Japan(69° S, 39° E)
Trinidad Head, USA(41° N, 124° W)
Tsukuba, Japan(36° N, 140° E)
Utö, FINLAND(59° N, 21° E)
Vindeln, SWEDEN(64° N, 19° E)
Virolahti, FINLAND(60° N, 27° E)
Westerland, GERMANY(54° N, 8° E)
Yonagunijima, Japan(24° N, 123° E)
Zingst, GERMANY(54° N, 12° E)
Zavodnje, Slovenia(46° N, 15° E)
Month
OBS
CB05
MOGUNTIA

2. CO


(a)
Alert,
Canada(82° N, 62° W)
(b)
Bukit Koto Tabang,
Indonesia(0° S, 100° E)
(c)
Candle Lake,
Canada(53° N, 104° W)
(d)
Cape Point,
South Africa(34° S, 18° E)
(e)
Cape Point,
South Africa(34° S, 18° E)
(f)
Cape Verde Observatory,
Cape Verde(16° N, 24° W)
(g)
Egbert,
Canada(44° N, 79° W)
(h)
East Trout Lake,
Canada(54° N, 104° W)
(i)
Fraserdale,
Canada(49° N, 81° W)
(j)
Hohenpeissenberg,
Germany(47° N, 11° E)
(k)
Jungfraujoch,
Switzerland(46° N, 7° E)
(l)
Kollumerwaard,
The Netherlands(53° N, 6° E)
(m)
Krvavec,
Slovenia(46° N, 14° E)
(n)
Mt. Kenya,
Kenya(0° S, 37° E)
(o)
Minamitorishima,
Japan(24° N, 153° E)
(p)
Payerne,
Switzerland(46° N, 6° E)
(q)
Rigi,
Switzerland(46° N, 8° E)
(r)
Ryori,
Japan(39° N, 141° E)
(s)
Schauinsland,
Germany(47° N, 7° E)
(t)
Sable Island,
Canada(43° N, 60° W)
(u)
Yonagunijima,
Japan(24° N, 123° E)
CO (ppb)
Month
J F M A M J J A S O N D
OBS
CB05
MOGUNTIA

3. O_3: EBI vs KPP



4. CO: EBI vs KPP