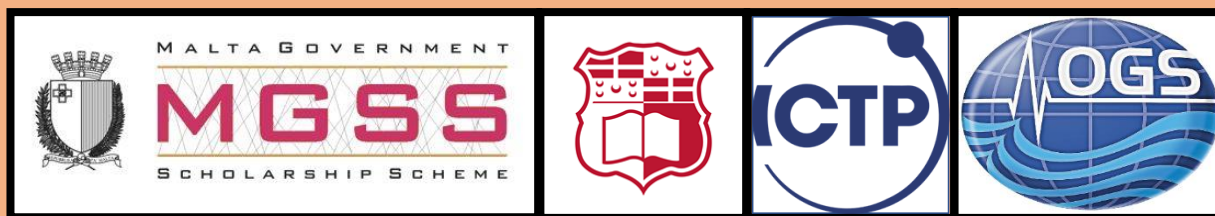


# A New Gas-Phase Scheme for Advanced Regional Climate Modelling with RegCM4

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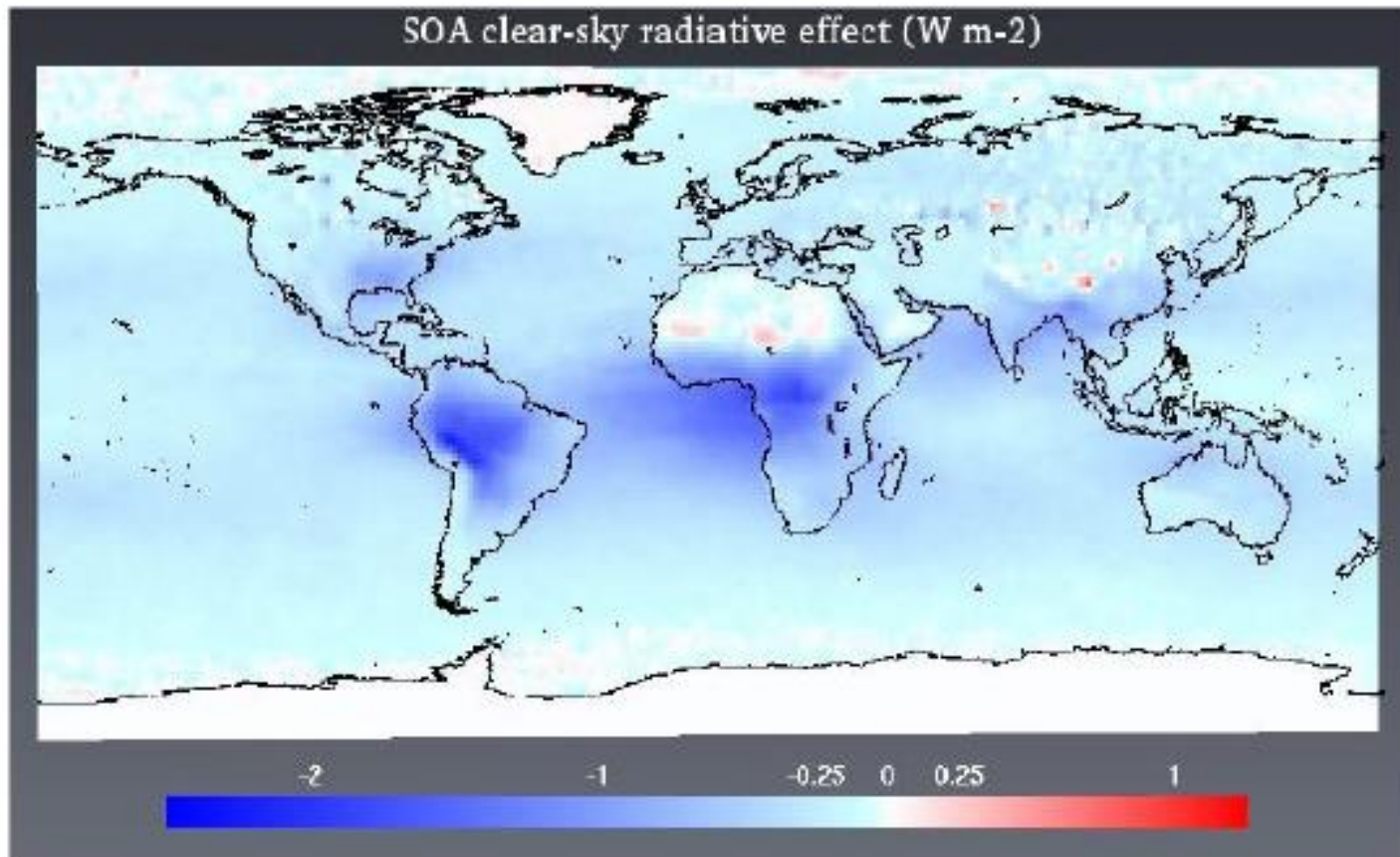
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International Workshop on ICTP Regional Climate Model:  
Applications over South Asia CORDEX Domain

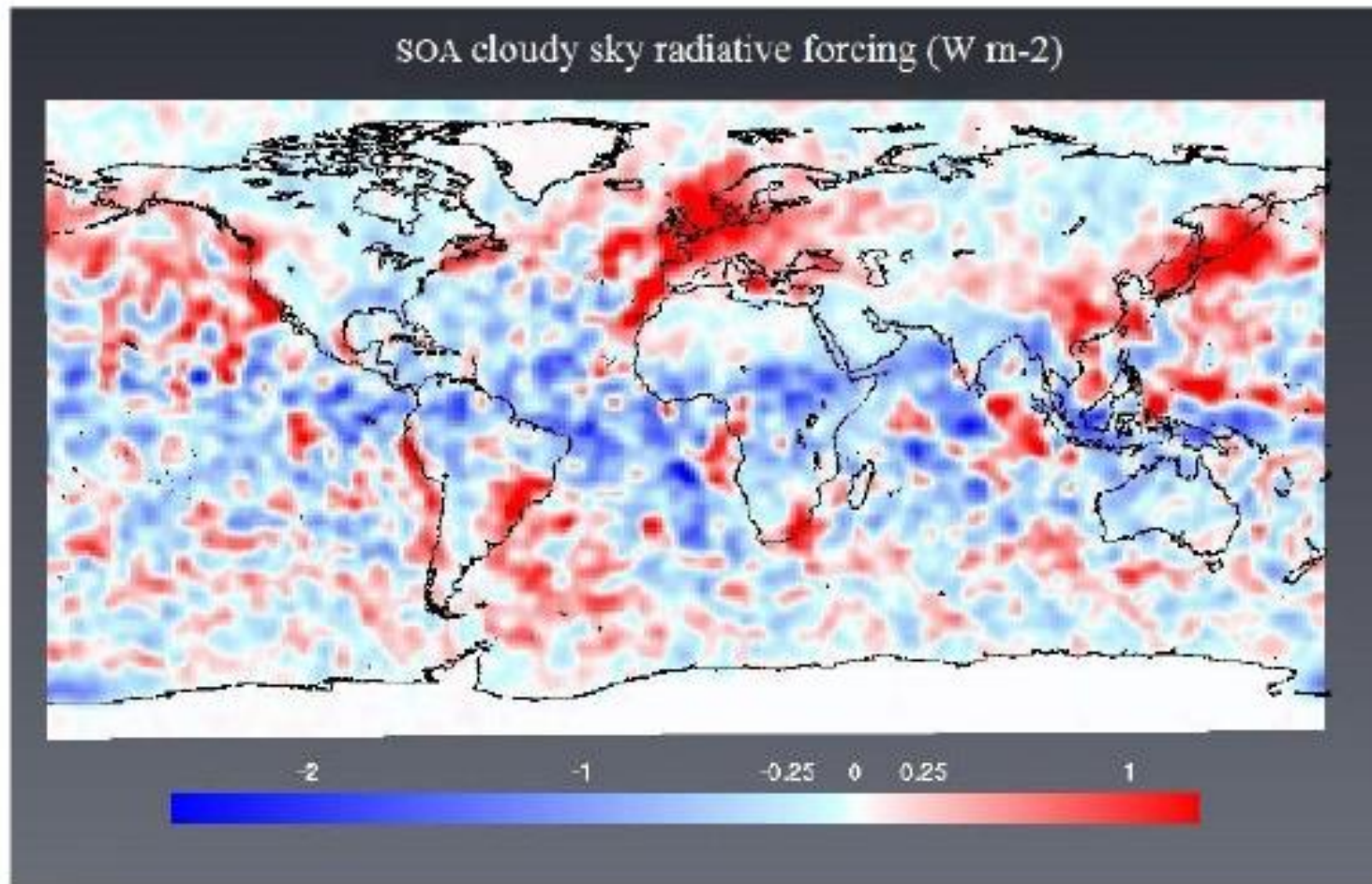
22-28 February 2021

# Motivation: Direct effects of SOAs



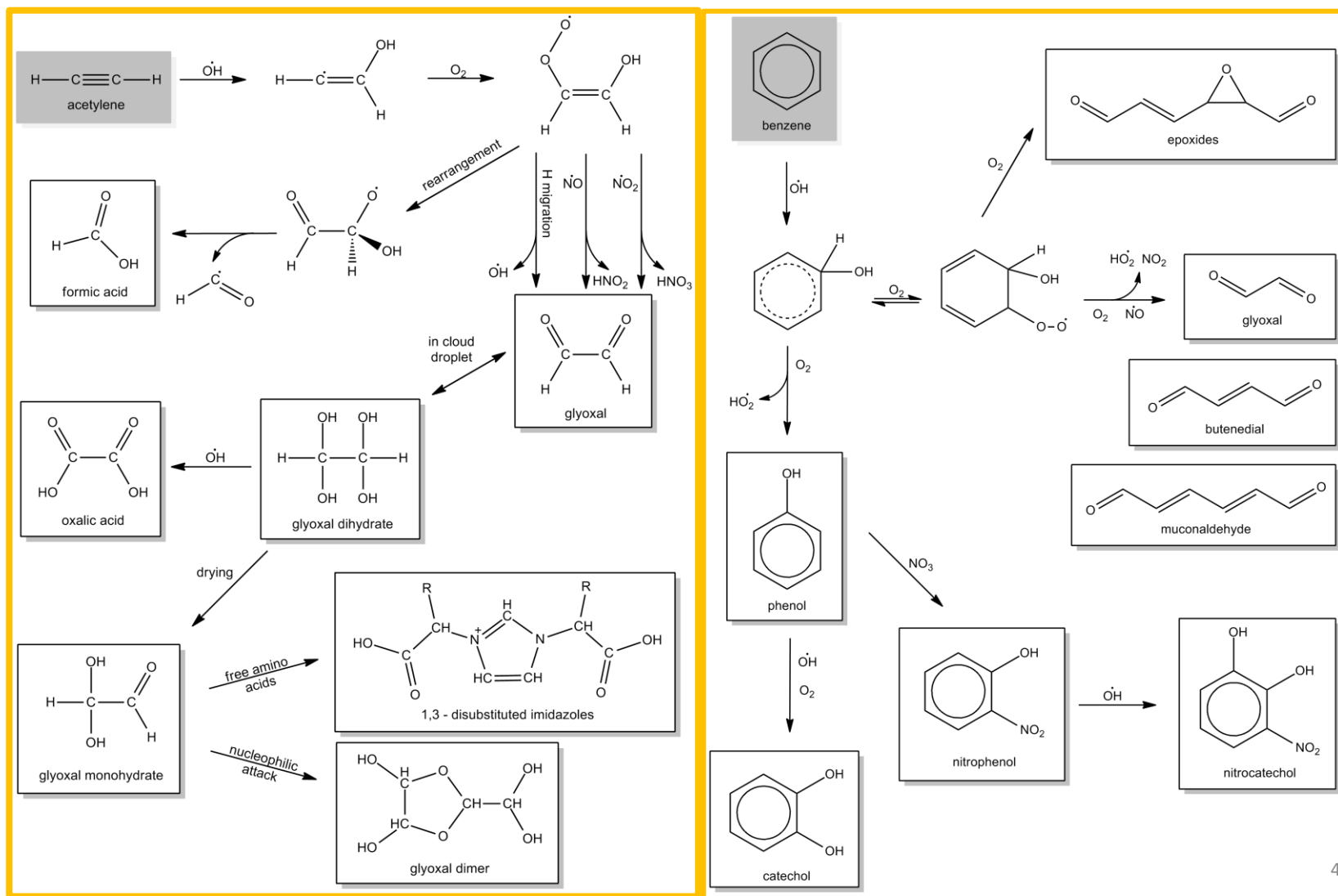
**Figure 1.4:** The annual direct SOA radiative forcing; obtained by calculating the difference in clear-sky top of atmosphere Sw flux between SOA and no SOA (O'Donnell *et al.*, 2011).

## Motivation: Indirect effects of SOAs

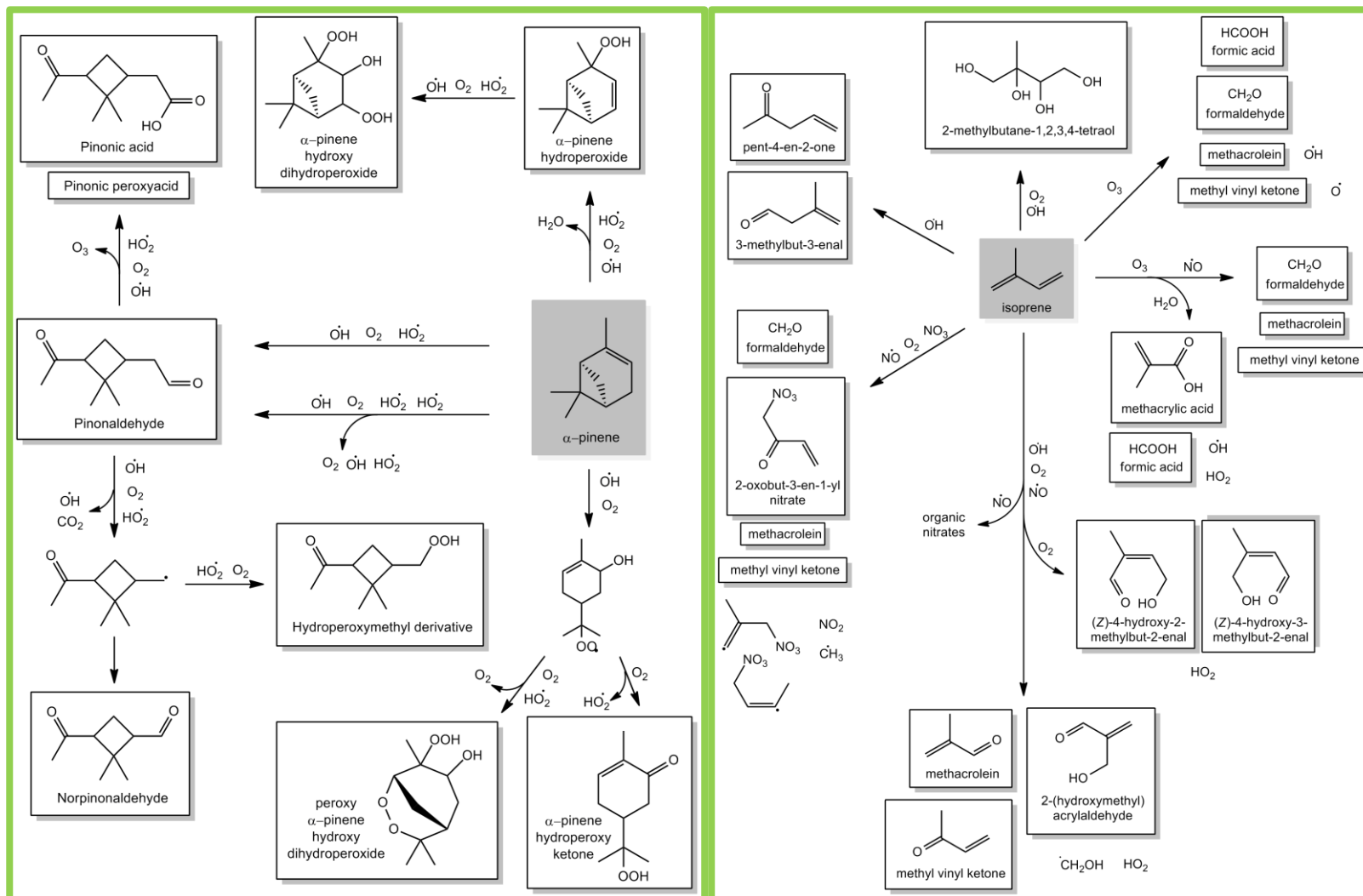


**Figure 1.5:** The annual indirect SOA radiative forcing; obtained using cloudy-sky radiative forcing (O'Donnell *et al.*, 2011). 3

# Gas-Phase reactions: Anthropogenic sources



# Gas-Phase reactions: Biogenic sources





# CB6-C Gas-Phase Scheme in RegCM4

	CBM-Z	CB6-C
variable species	57	77
reactions	124	216

- alternative to CBM-Z (Shalaby et al., 2012; Zaveri and Peters, 1999)
- Based on Carbon Bond Mechanism 6 (rev 2)  
(Yarwood et al., 2012; Ruiz and Yarwood, 2013; Goldberg et al., 2016)
- Reactions:
  - 95 similar chemical reactions;
  - additional isoprene products;
  - new oxidation mechanisms for formic acid.
- new chemical species:
  - pentane, ethyne, ethanol, acetic acids, methyl ethyl ketone, glyoxal, glycolaldehyde, benzene, nitrocresol, methacrolein, epoxides, and monoterpenes.

- **Chemical Boundary Conditions**

- Model for Ozone and Related chemical Tracers (MOZART)
- Climatology 1999-2009
- Emmons et al. (2009)

CB6-C	MOZART data	Mf
Propane	Propane	3
Isoprene	Isoprene	0
Methacrolein	(Methyl vinyl ketone +Methacrolein+Hydroxycarbonyl)	4
Glycolaldehyde	Glycolaldehyde	4
Multifunc. nitrates	Organic nitrates	1
Isoprene nitrates	Isoprene+NO3 peroxy radical	1
Benzene	Toluene	0.29
Ethanol	Ethanol	1
Pinene	Pinene	1

- **Emissions**

- International Institute for Applied System Analysis (IIASA)
- global emission database 1990 to 2010
- Lamarque et al. (2010)

- **Photolysis Rates**

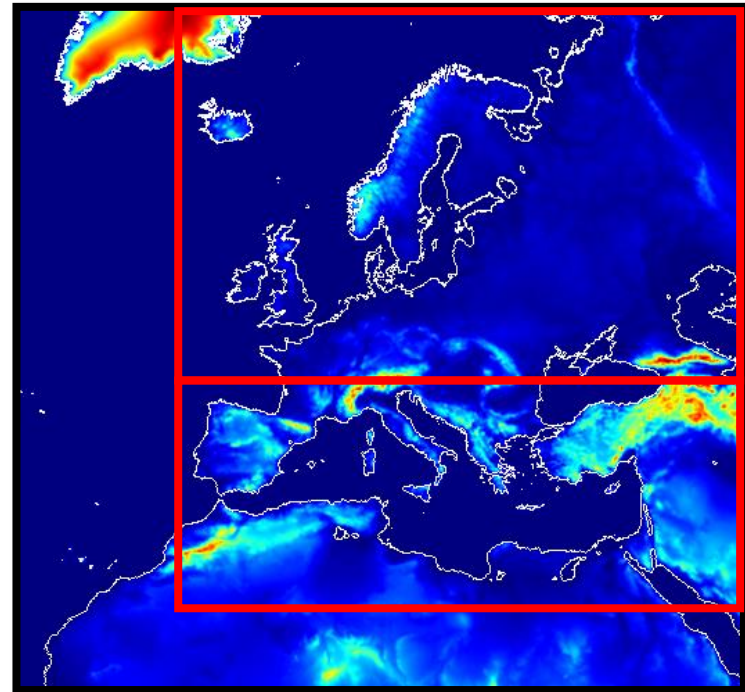
- Madronich Tropospheric Ultraviolet (TUV) scheme
- Madronich and Flocke (1999), Tie et al. (2003).
- photolytic rates were assumed to be equal (or very similar) for chemicals with a similar composition

CB6-C		J-val Source			
C3+ Peroxyacyl nitrate		Peroxyacyl nitrate	CB6-C	IIASA data	Mf
Butyl hydroperoxide		Methylhydroperoxide	Butene	Internal Olefins	7
Glycolaldehyde		Methacrolein	Isoprene	Isoprene	0.05
Methyl ethyl ketone		Acetone	Ethyne	Ethene	1.12
(Z)-4-Hydroperoxy-3-methyl-2-butenal		Methylhydroperoxide	Ethanol	Ethene	0.82
Nitro-cresols		Hydroxy/Alkyl nitrates	Benzene	Toluene	0.29
2-Pentenedial		Glyoxal	Pinene	Isoprene	0.2
Butenedial		Glyoxal			



# Domain & Simulation

- **Resolution:** 50 km
- **Chem Data:** MZCLM
- **SST data:** Weekly OISST
- **ICBC data:** NCEP/NCAR Reanalysis
- Time Period: 2003-2005
- Sub-regions:
  - Northern: 45 to 75 N
  - Southern: 30 to 45 N
- ICTP cluster 'Argo'
  - 60 (3 x20) processors
  - 63Gb memory

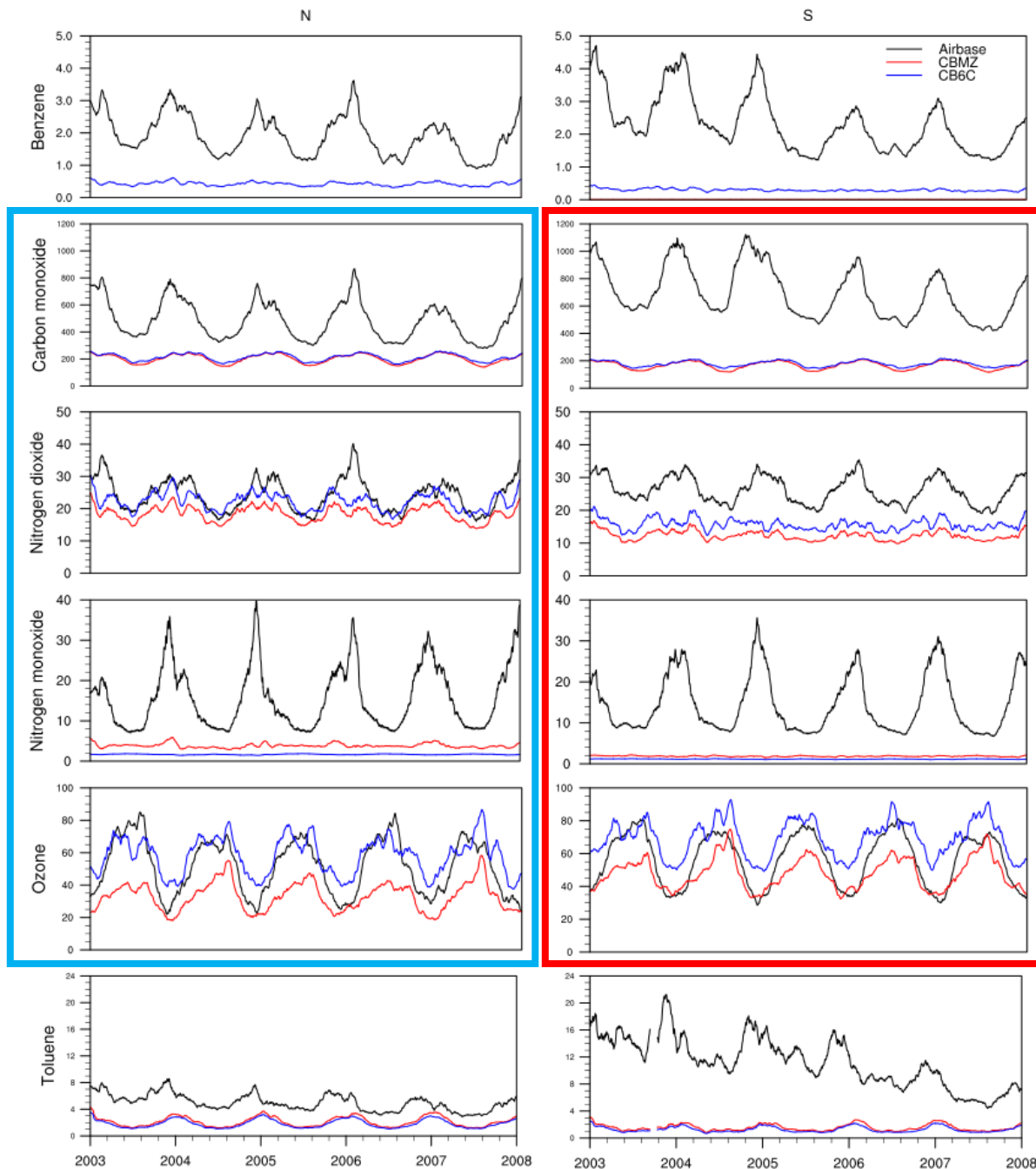


	CBM-Z	CB6-C	CB6-C Change
Sim. Time [/mon]	1.400 hr	2.092 hr	49.4 % slower
Output [/mon]	6.3 GB	9.4 GB	49.2 % bigger

# Stations

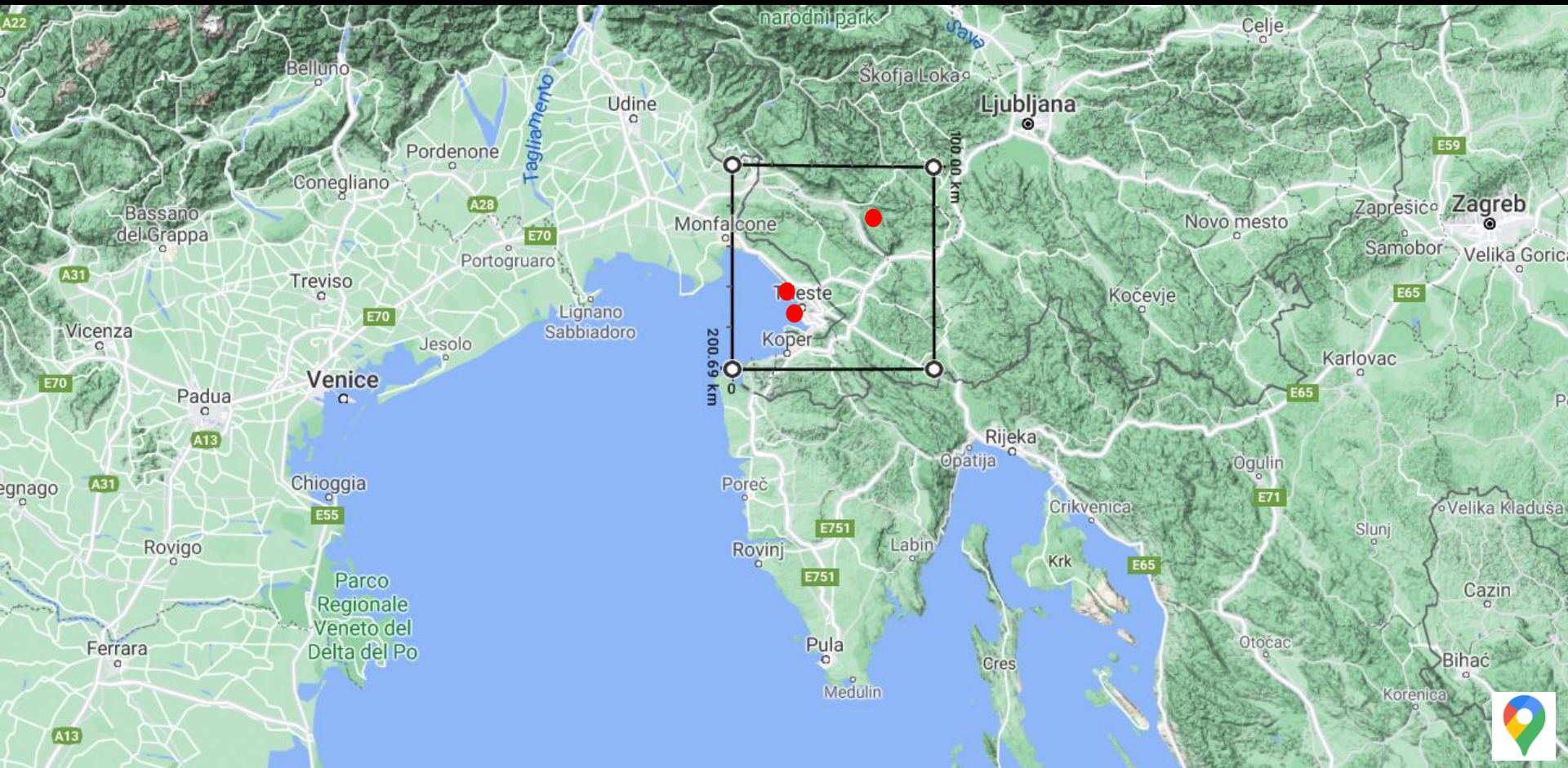
- European Air quality Database (AirBase) station data
- Number of stations

Chemical Species	N Min	N Mean	N Max	S Min	S Mean	S Max
Benzene	106	158.3	190	24	69.4	120
<b>Carbon monoxide</b>	<b>381</b>	<b>418.9</b>	<b>452</b>	<b>145</b>	<b>217.3</b>	<b>293</b>
<b>Nitrogen dioxide</b>	<b>801</b>	<b>927.3</b>	<b>1003</b>	<b>232</b>	<b>346.8</b>	<b>452</b>
<b>Nitrogen monoxide</b>	<b>401</b>	<b>523.3</b>	<b>643</b>	<b>140</b>	<b>245.2</b>	<b>349</b>
<b>Ozone</b>	<b>792</b>	<b>885.2</b>	<b>945</b>	<b>251</b>	<b>348.0</b>	<b>435</b>
Toluene	49	60.2	73	0	24.2	55

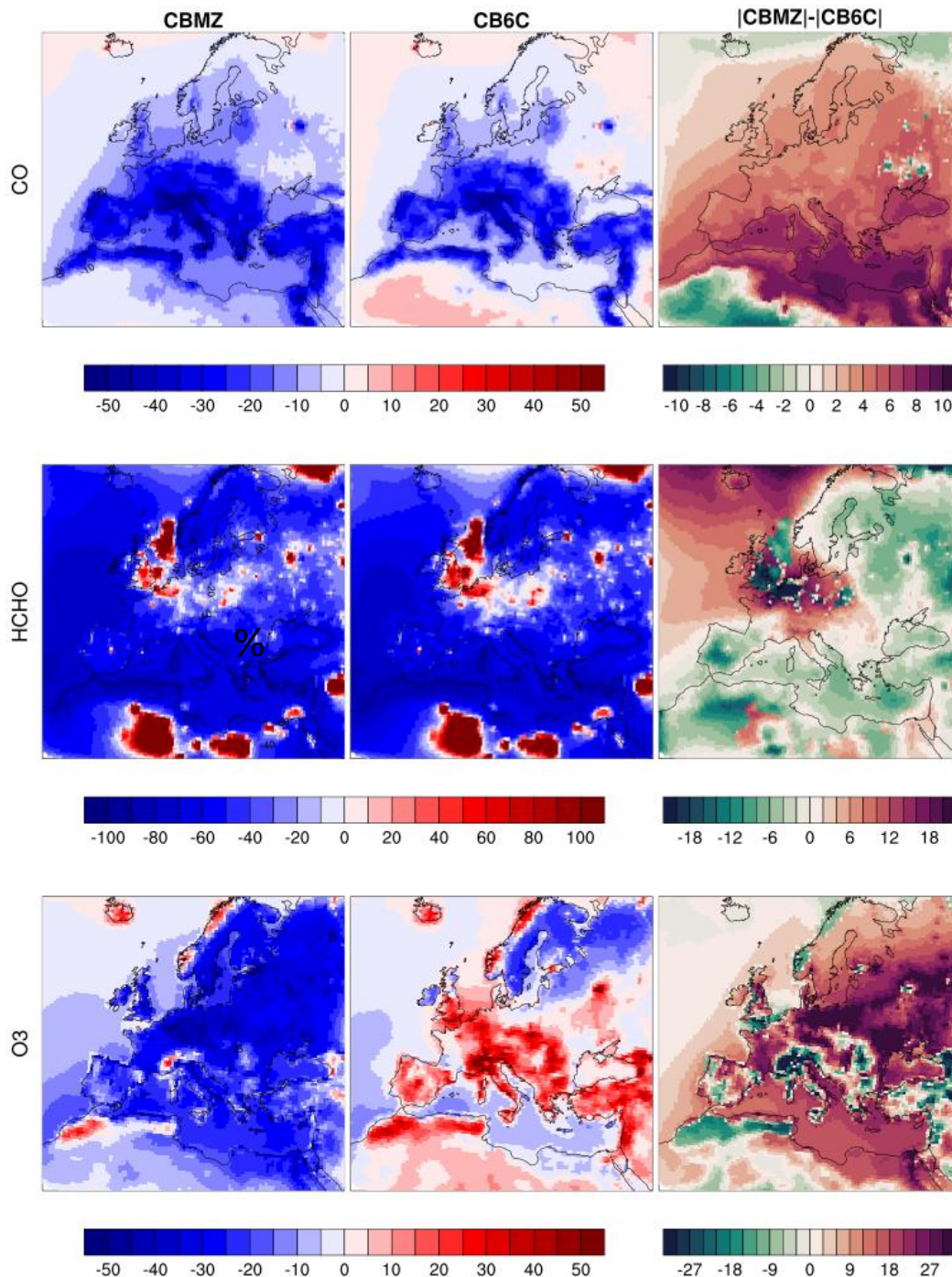


Inter-annual variability for surface concentration ( $\mu\text{g}/\text{m}^3$ ) compared to the mean of all AirBase stations.

# Comparing stations with grid-cells

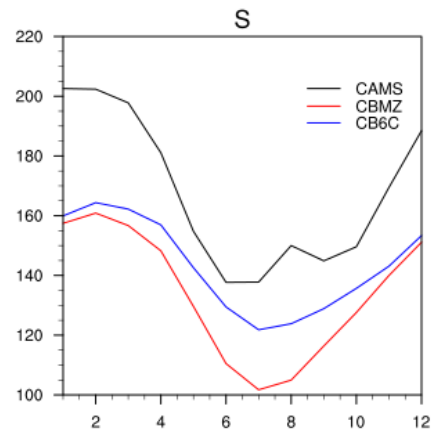
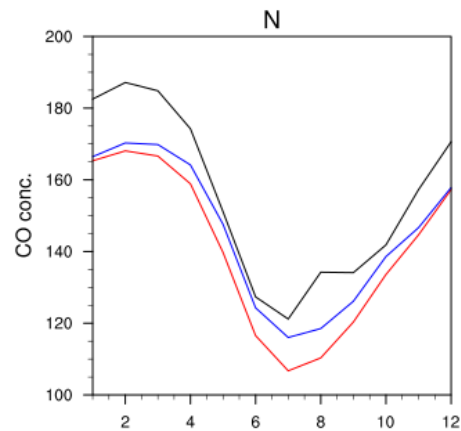




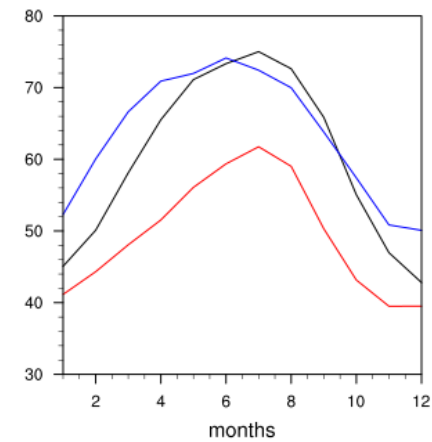
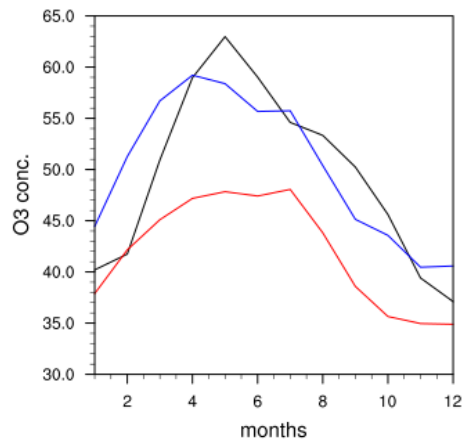
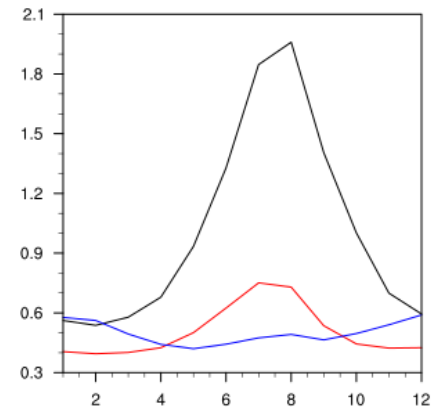
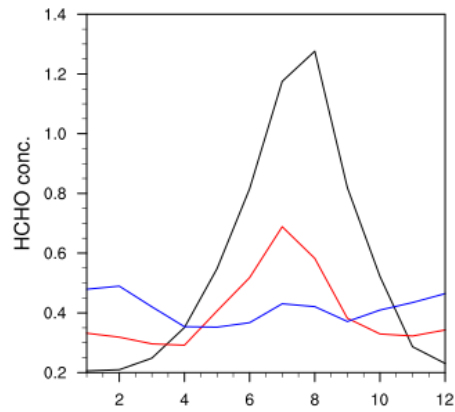


Relative bias (%) of the surface mixing ratio annual mean compared to CAMS data (Inness et al., 2019).

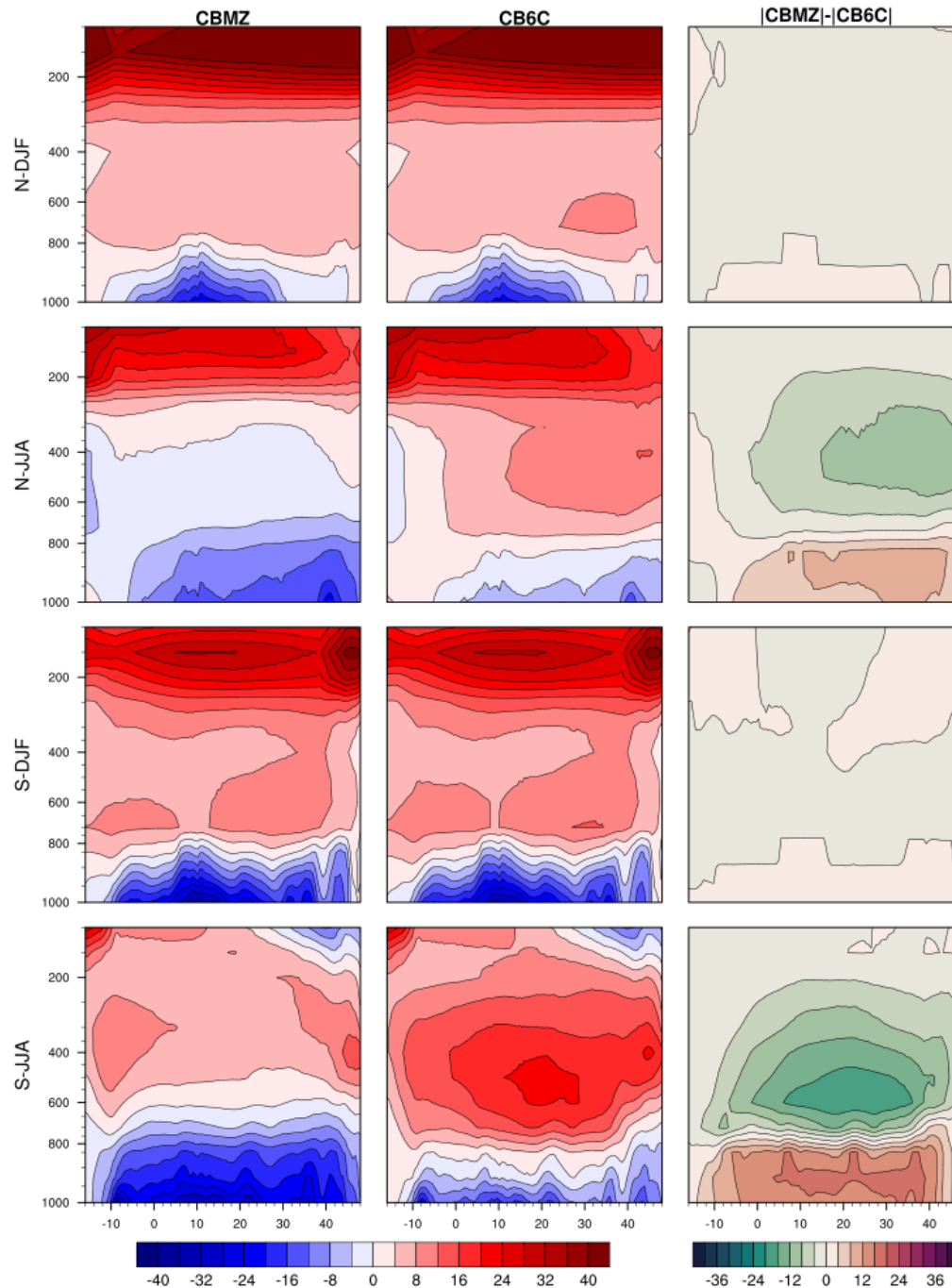
The right-most column shows the differences (%) between the absolute biases of the two models.



Annual cycle of surface concentration (ppb) spatial means compared to CAMS data.



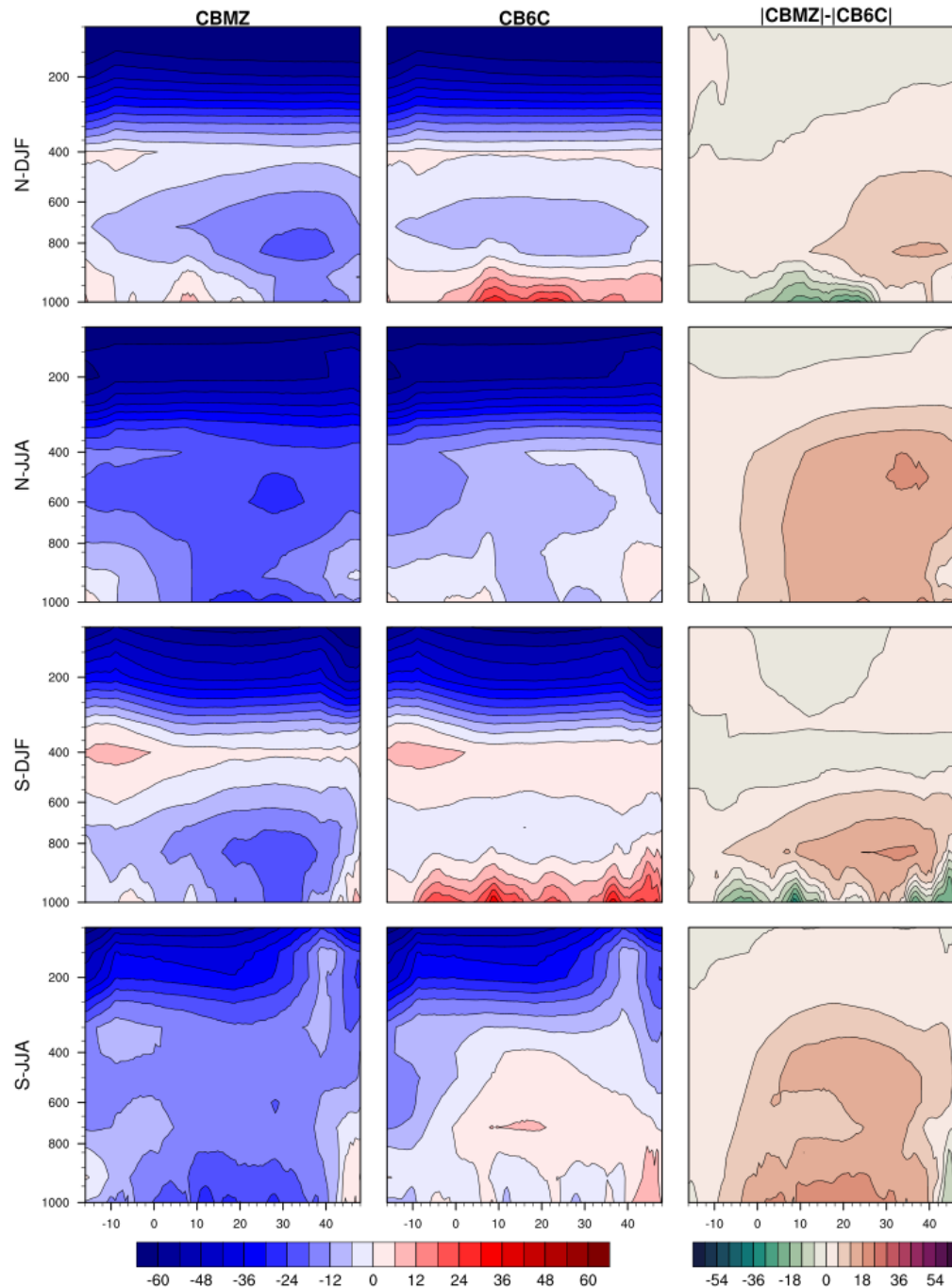




Relative bias (%) of the vertical meridional means of carbon monoxide.

The right-most column shows the differences (%) between the absolute biases.

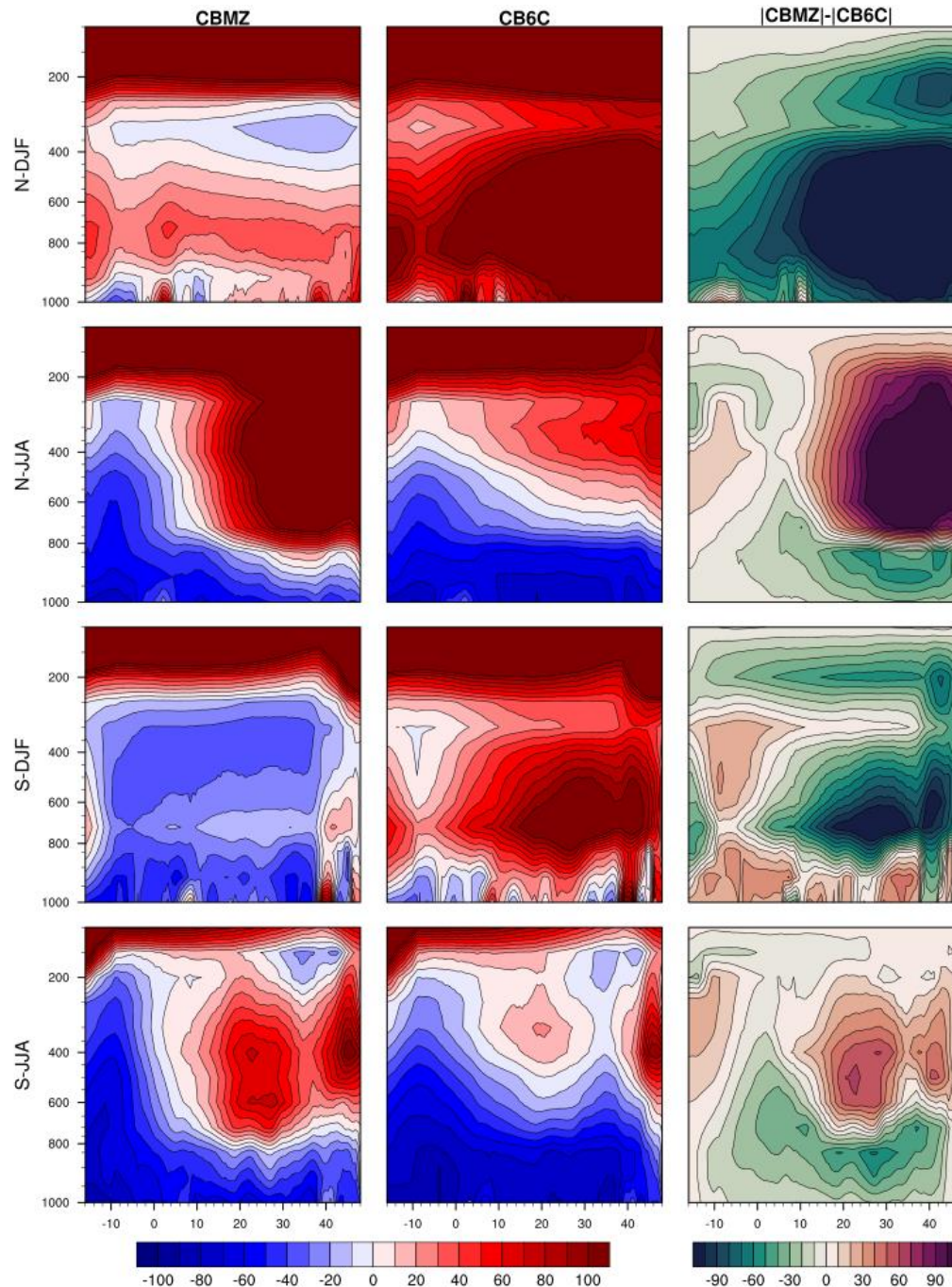
The pressure levels are expressed in hPa.



Relative bias (%) of the vertical meridional means of ozone.

The right-most column shows the differences (%) between the absolute biases.

The pressure levels are expressed in hPa.



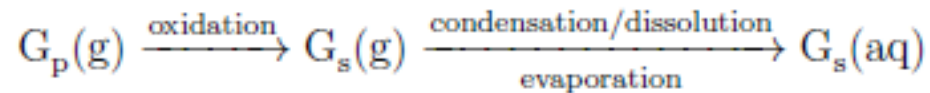
Relative bias (%) of the vertical meridional means of formaldehyde.

The right-most column shows the differences (%) between the absolute biases.

The pressure levels are expressed in hPa.

# Conclusions

- Model is operational with reliable O<sub>3</sub> and CO products
- Formaldehyde and organic products require further tuning
  - Additional testing in progress...
- Next Step: Activation of SOA Module



- Source:
  - Ciarlo` JM, et al. (*in review*). A Modified Gas-Phase Scheme for Advanced Regional Climate Modelling with RegCM4. Climate Dynamics.
- Model available at:
  - <https://github.com/ciarloj/RegCM4.5-CB6C>
  - Tutorial starting shortly...



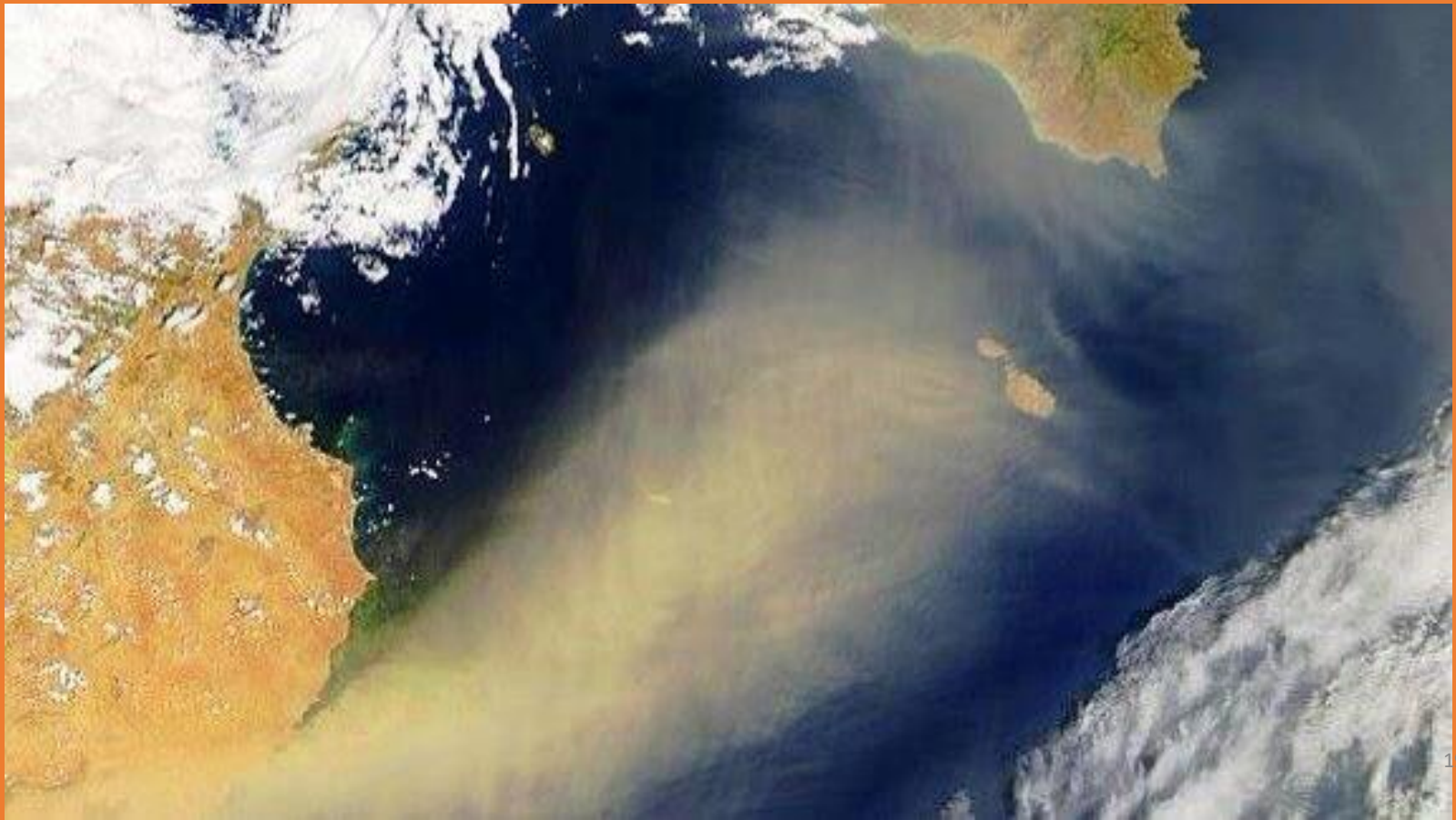


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SCHOLARSHIP SCHEME



# Thank You

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# References

- Emmons LK et al (2009) Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4). Geoscientific Model Development Discussions 2(2):1157{1213, DOI 10.5194/gmdd-2-1157-2009.
- Goldberg DL et al (2016) CAMx ozone source attribution in the eastern United States using guidance from observations during DISCOVER-AQ Maryland. Geophysical Research Letters 43(5):2249{2258, DOI 10.1002/2015GL067332.
- Inness A et al (2019) The CAMS reanalysis of atmospheric composition. Atmospheric Chemistry and Physics 19(6):3515{3556, DOI 10.5194/acp-19-3515-2019.
- Lamarque JF et al (2010) Historical (1850-2000) gridded anthropogenic and biomass burning emissions of reactive gases and aerosols: Methodology and application. Atmospheric Chemistry and Physics. 10(15):7017{7039, DOI 10.5194/acp-10-7017-2010
- Madronich S, Flocke S (1999) The Role of Solar Radiation in Atmospheric Chemistry. In: Boule P (ed) Handbook of Environmental Chemistry, January 1998, pp 1{26, DOI 10.1007/978-3-540-69044-3\_1
- O'Donnell D et al (2011). Estimating the direct and indirect effects of secondary organic aerosols using ECHAM5-HAM. Atmospheric Chemistry and Physics 11(16):8635{8659.
- Ruiz LH, Yarwood G (2013) Interactions between Organic Aerosol and Noy: Influence on Oxidant Production. Prepared for the Texas AQRP (Project 12-012). Tech. rep., The University of Texas at Austin
- Shalaby A, et al (2012) Implementation and evaluation of online gas phase chemistry within a regional climate model (RegCM-CHEM4). Geoscientific Model Development 5(3):741-760, DOI 10.5194/gmd-5-741-2012
- Tie X, Madronich S, Walters S, Zhang R, Rasch P, Collins W (2003) Effect of clouds on photolysis and oxidants in the troposphere. Journal of Geophysical Research 108(D20):4642, DOI 10.1029/2003JD003659
- Yarwood G, et al (2012) Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms AQRP Project 10-042. Tech. rep., The University of Texas at Austin
- Zaveri Ra, Peters LK (1999) A new lumped structure photochemical mechanism for large-scale applications. Journal of Geophysical Research 104(D23):30387, DOI 10.1029/1999JD900876