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Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

The multiscale NMMB/BSC Chemical Transport Model: developments of inlined aerosol and gas chemistry processes

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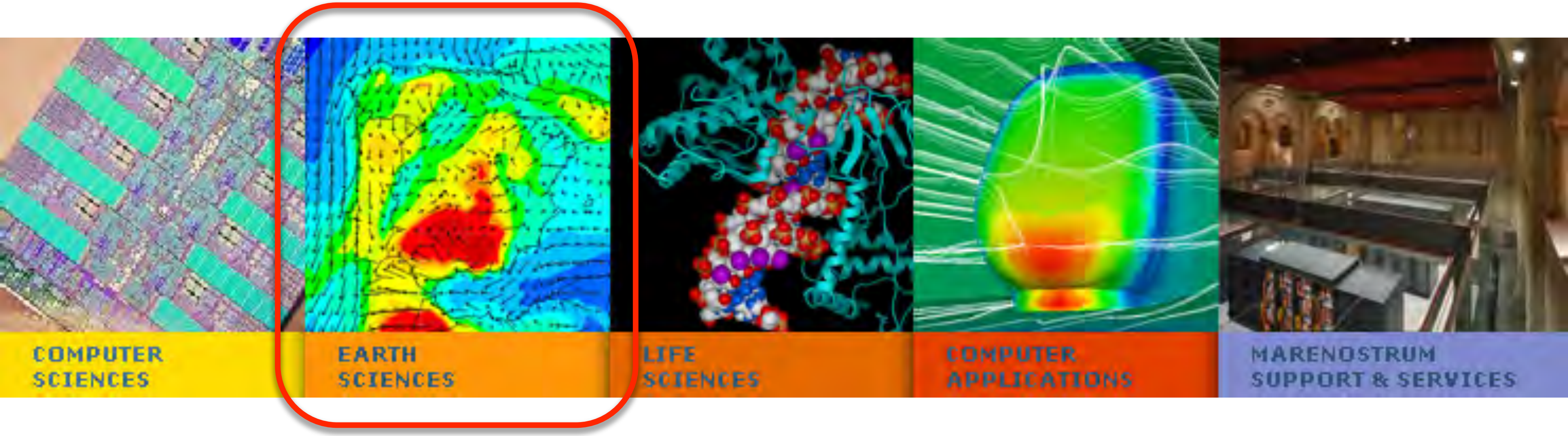
Acknowledgments: Z. Janjic, T. Black, C. Pérez, S. Basart, A. Badia, M. Spada, J.M. Baldasano, D. Dabdub, K. Haustein, M. Carreras, E. Tarradellas, F. Benicasa

Severo-Ochoa Seminar, Barcelona, October 25, 2013

BSC Departments

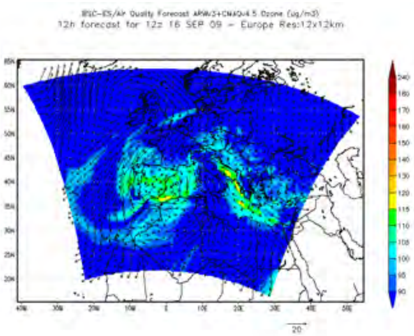


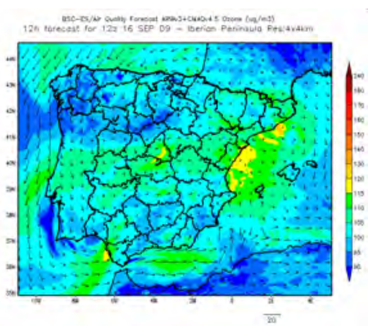
The Earth Sciences Department is devoted to the development and implementation of regional and global state-of-the-art models for air quality, meteorology and climate applications

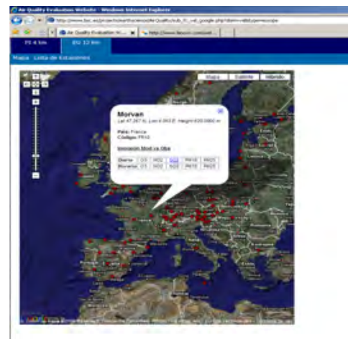
ES air quality modelling activites

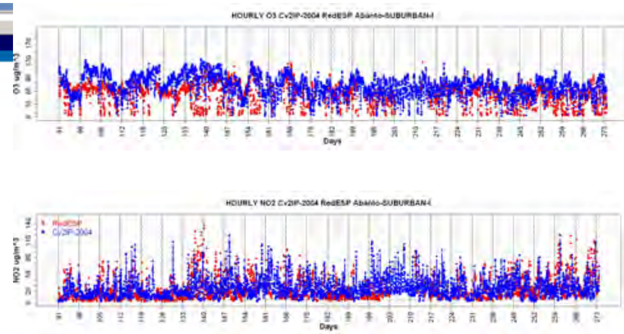
CALIOPE daily forecast and near-real time verification

✓ Daily experimental forecasts for meteorology and air quality (12 km for Europe and 4 km for the Iberian Peninsula) (http://www.bsc.es/caliope).



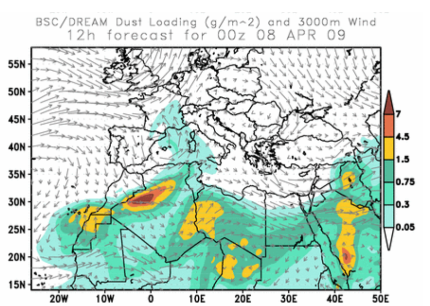


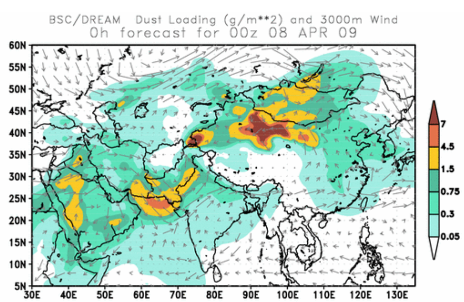


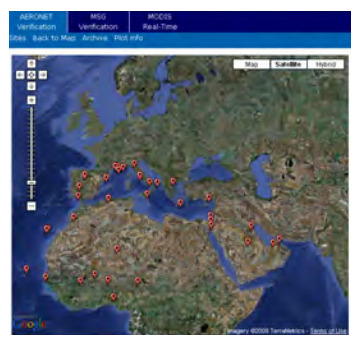


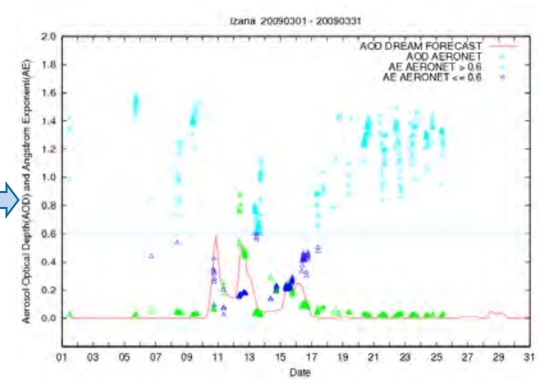
BSC/DREAM and NMMB/BSC-Dust daily forecast and verification

North Africa/Mediterranean - 1/3 x 1/3 degree resolution
Asia domain - 1/2 x 1/2 degree resolution



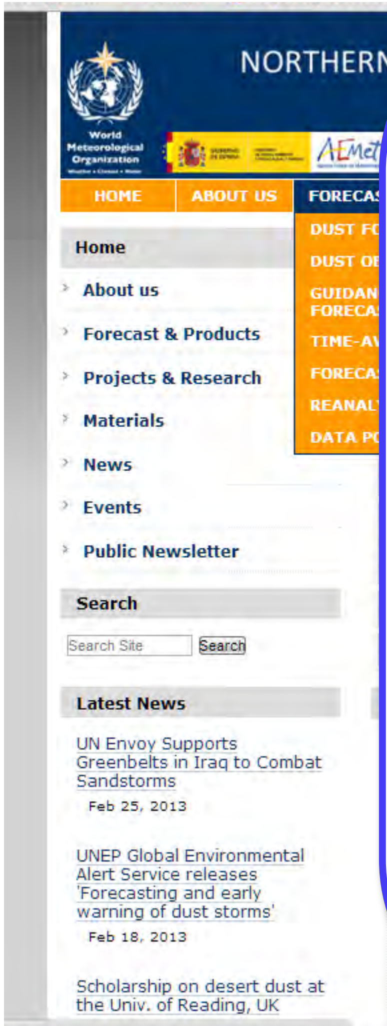


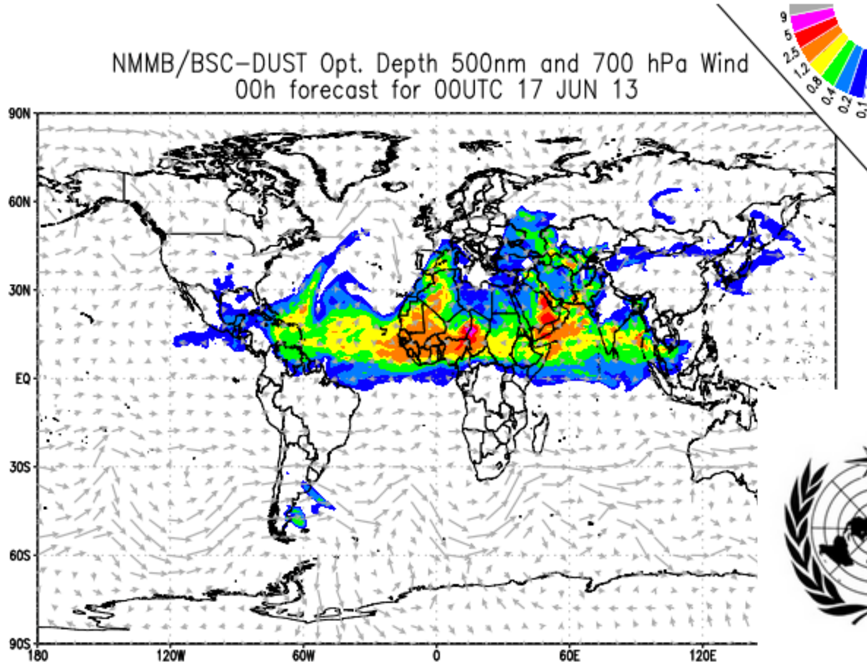




→ http://www.bsc.es/earth-sciences/mineral-dust-forecast-system/bsc-dream8b-forecast/

SDS-WAS NA-ME-E RC: http://sds-was.aemet.es





First Specialized Center for Mineral Dust Prediction of the World Meteorological Organization

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warning to
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sdswas@aemet.es

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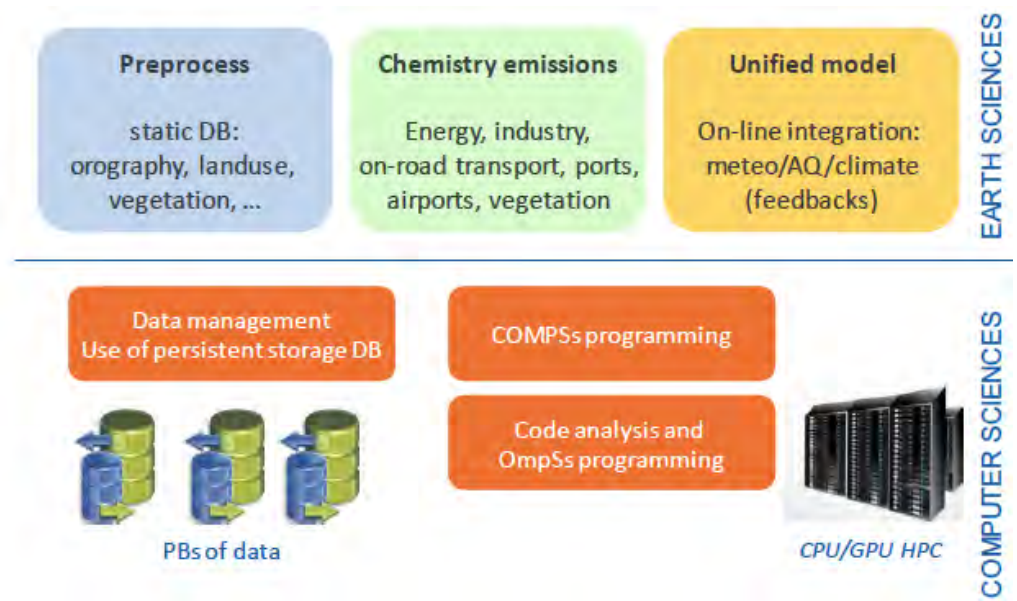
Severo-Ochoa Earth Sciences Application

- Development of Unified Meteorology/Air Quality/Climate model
  - Towards global high-resolution system for global to local assessments



- Extending NMMB/BSC-CTM from coarse regional scales to global high-resolution configurations
- Extending short-term applications to climate scales

- International collaborations:

Meteorology

National Centers for Environmental Predictions

Climate
Global aerosols

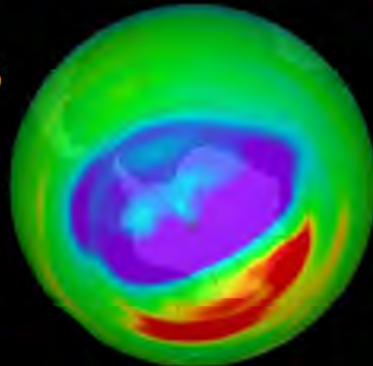
Goddard Institute Space Studies

Air Quality

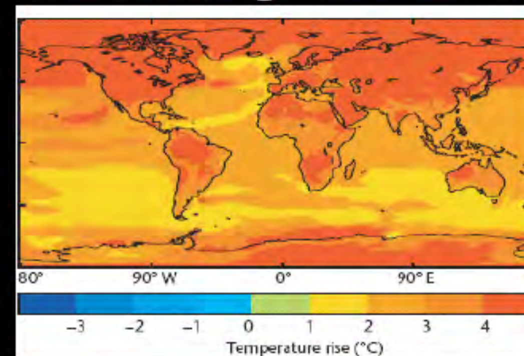
Uni. of California Irvine

Combining Air Chemistry, Meteorology and Climate Research

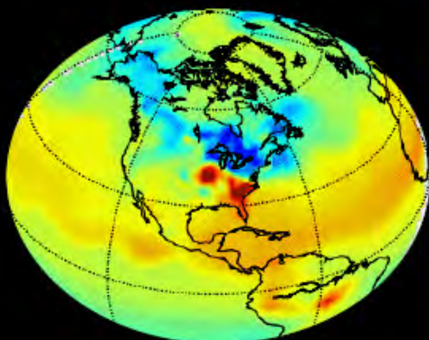
O_3



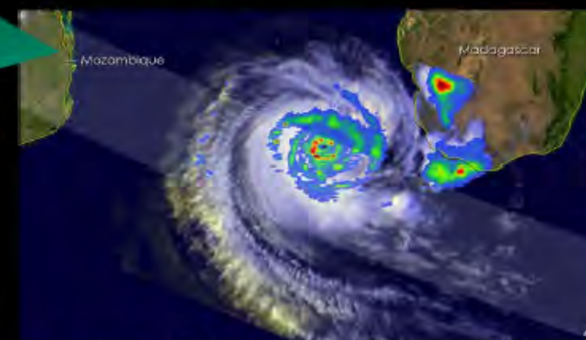
Climate Change & Prediction



GHGs

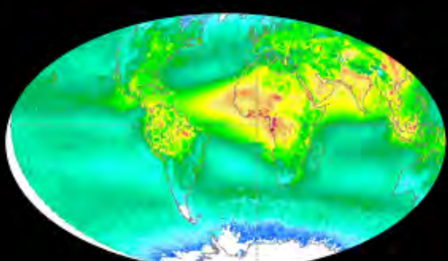


Weather Prediction



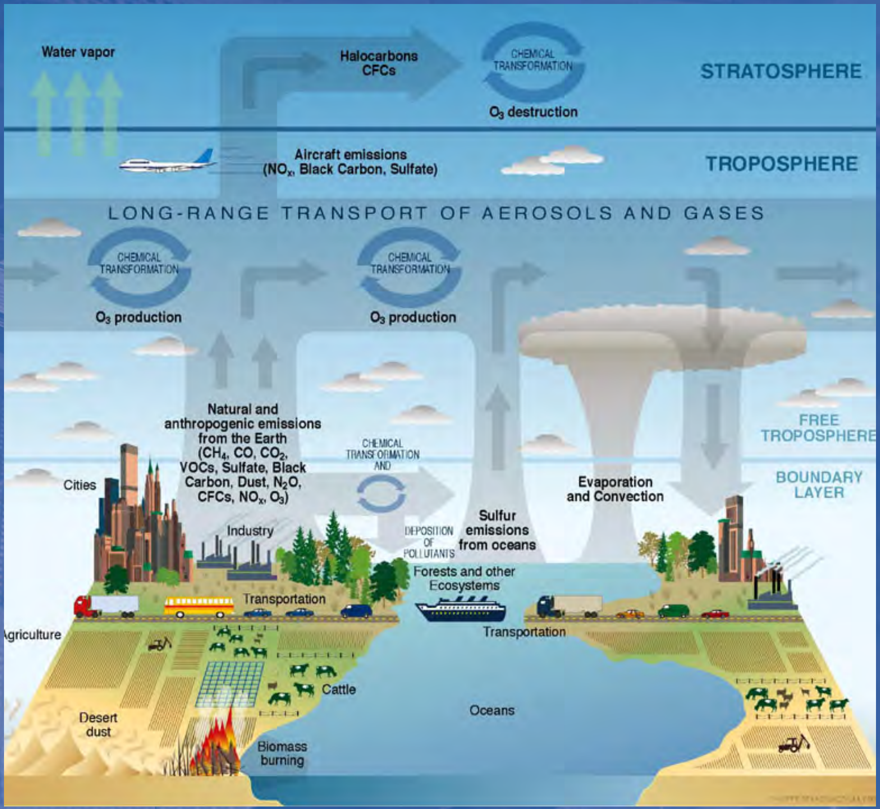
Process Studies
Modelling
Observations

Aerosols & Dust



Severe Storms

Air Pollution



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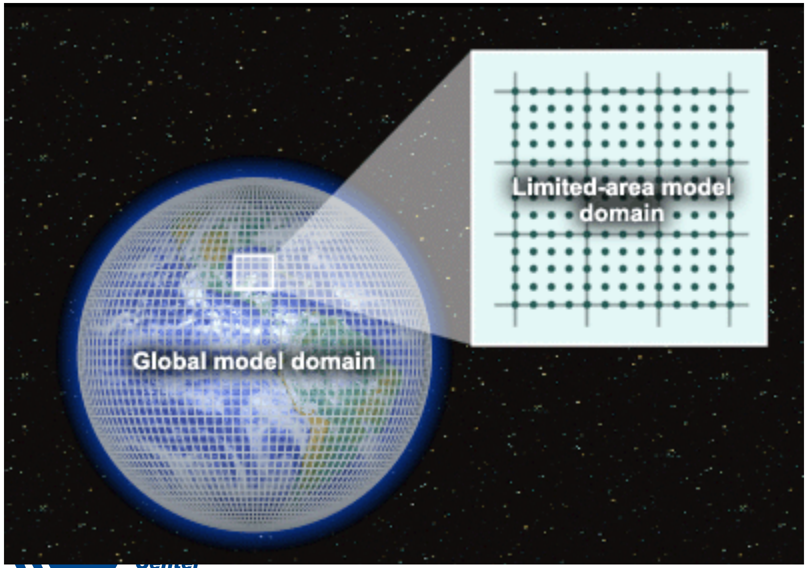
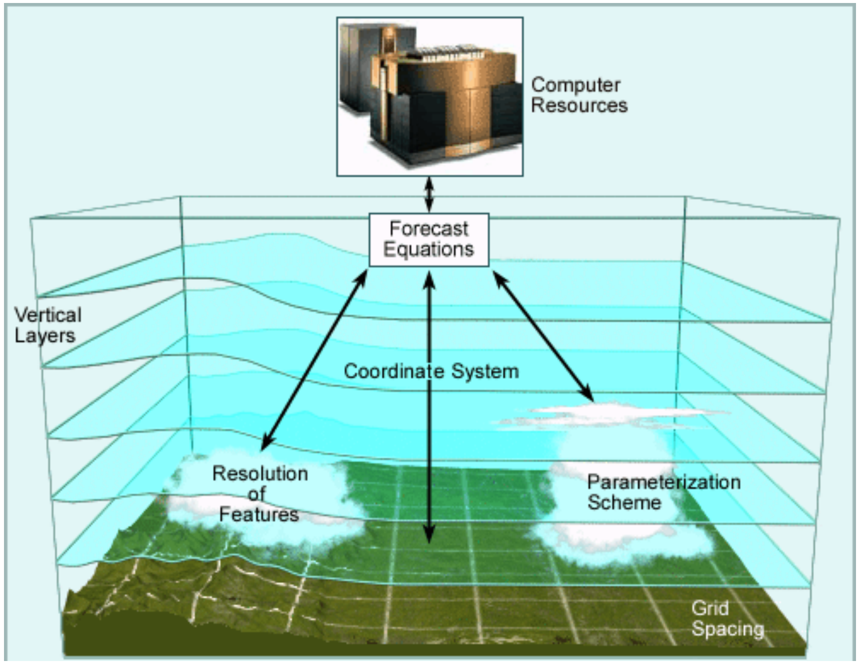
NMMB/BSC CHEMICAL TRANSPORT MODEL

Main model framework

- The Nonhydrostatic Multiscale Meteorological Model on the B grid (NMMB)
- Developed at National Centers for Environmental Prediction (NCEP)

- ***Multiscale*** (global to regional) and ***Nonhydrostatic*** (up to 1km^2 horizontal resolution)





Model equations

METEOROLOGY CHEMISTRY ON-LINE INTERACTIONS TAKEN INTO CONSIDERATION BY NMMB/BSC-CTM MODEL AND ITS FUTURE DEVELOPMENTS

$$\partial_t Q_{i,j} + (\vec{v}\cdot\vec{\nabla}) Q_{i,j} = \sum_k \frac{dQ_{i,j}}{dt}(u^*, \vec{q}_w, \vec{c}_g, \ldots)\Big|_{aero,k}$$

$$\partial_t \rho_{d,a} + \vec{\nabla}(\rho_{d,a}\vec{v}) = 0$$

$$\partial_t \vec{v} + (\vec{v}\cdot\vec{\nabla})\vec{v} = -f\vec{k}\times\vec{v} - \vec{\nabla}\Phi - \frac{1}{\rho_a}\vec{\nabla} p + \frac{d\vec{v}}{dt}\Big|_{turb}$$

$$\partial_t T + (\vec{v}\cdot\vec{\nabla}) T = \sum_k \frac{dT}{dt}(I_\lambda, \ldots)\Big|_{diab,k} + \frac{dT}{dt}\Big|_{turb}$$

$$\partial_t q_{w,n} + (\vec{v}\cdot\vec{\nabla}) q_{w,n} = \sum_k \frac{dq_{w,n}}{dt}\Big|_{water,k}$$

$$p\alpha = RT$$

$$\partial_t c_{g,y} + (\vec{v}\cdot\vec{\nabla}) c_{g,y} = \frac{dc_{g,y}}{dt}(\vec{c}_g, I_\lambda, \ldots)\Big|_{photochem,k} + \ldots$$

$$\frac{dI_\lambda}{dt} = f(I_\lambda, \tau_\lambda^{aero}, \omega_\lambda^{aero}, g_\lambda^{aero}, \ldots)$$

Radiative Transfer Eq.

Resolving the full compressible primitive equations:

Mass conservation

Momentum conservation

Energy conservation

Moisture conservation

Gas – aerosol conservation

The chemical term: chemical mechanism

Reaction Number	Reaction	Rate Constant, $k^{\dagger}$	Note
	Inorganic Chemistry		
(1)	$NO_2 + h\nu \xrightarrow{O_2} NO + O(^3P)$	J_{NO_2}	
(2)	$NO_3 + h\nu \longrightarrow 0.89NO_2 + 0.89O(^3P) + 0.11NO$	J_{NO_3}	
(3)	$HNO_2 + h\nu \longrightarrow OH + NO$	J_{HNO_2}	
(4)	$HNO_3 + h\nu \longrightarrow OH + NO_2$	J_{HNO_3}	
(5)	$HNO_4 + h\nu \longrightarrow HO_2 + NO_2$	J_{HNO_4}	
(6)	$O_3 + h\nu \longrightarrow O(^3P)$	J_{O_3a}	
(7)	$O_3 + h\nu \longrightarrow O(^1D)$	J_{O_3b}	
(8)	$H_2O_2 + h\nu \longrightarrow 2OH$	$J_{H_2O_2}$	
(9)	$O(^1D) + O_2 \longrightarrow O(^3P) + O_2$	3.2×10^{-11} exp (70	
(10)	$O(^1D) + N_2 \longrightarrow O(^3P) + N_2$	1.8×10^{-11} exp (11	
(11)	$O(^1D) + H_2O \longrightarrow 2OH$	2.2×10^{-10}	
(12)	$O(^3P) + O_2 \xrightarrow{M} O_3$	F(6.0(-34), 2.3, 0.0	
(13)	$O(^3P) + O_3 \longrightarrow O_2 + O_2$	8.0×10^{-12} exp (−	
(14)	$O(^3P) + NO_2 \longrightarrow NO$	6.5×10^{-12} exp (−	
(15)	$O(^3P) + NO_2 \xrightarrow{M} NO_3$	F(9.0(-32), 2.0, 2.2	
(16)	$O(^3P) + NO \xrightarrow{M} NO_2$	F(9.0(-32), 1.5, 3.0	
(17)	$O_3 + NO \longrightarrow NO_2$	2.0×10^{-12} exp (−	
(18)	$O_3 + NO_2 \longrightarrow NO_3$	1.2×10^{-13} exp (−	
(19)	$O_3 + OH \longrightarrow HO_2$	1.6×10^{-12} exp (−	
(20)	$O_3 + HO_2 \longrightarrow OH$	1.1×10^{-14} exp (−	
(21)	$OH + H_2 \longrightarrow HO_2 + H_2O$	5.5×10^{-12} exp (−	
(22)	$OH + NO \xrightarrow{M} HNO_2$	F(7.0(-31), 2.6, 3.6	
(23)	$OH + NO_2 \xrightarrow{M} HNO_3$	F(2.5(-30), 4.4, 1.6	
(24)	$OH + NO_3 \longrightarrow HO_2 + NO_2$	2.2×10^{-11}	
(25)	$OH + HNO_2 \longrightarrow NO_2$	1.8×10^{-11} exp (−	
(26)	$OH + HNO_3 \xrightarrow{M} NO_3$	$k_a + [M]k_b/(1 + [M$ $k_a = 7.2 \times 10^{-15}$ e $k_b = 1.9 \times 10^{-33}$ e $k_c = 4.1 \times 10^{-16}$ e	
(27)	$OH + HNO_4 \longrightarrow NO_2$	1.3×10^{-12} exp (38	
(28)	$OH + HO_2 \longrightarrow H_2O + O_2$	4.8×10^{-11} exp (25	
(29)	$OH + H_2O_2 \longrightarrow HO_2$	2.9×10^{-12} exp (−	
(30)	$HO_2 + HO_2 \xrightarrow{M} H_2O_2$	$(k_d + [M]k_e)$ $k_d = 2.3 \times 10^{-13}$ e $k_e = 1.7 \times 10^{-33}$ e	
(31)	$HO_2 + HO_2 + H_2O \xrightarrow{M} H_2O_2$	$k_{30} \times 1.4 \times 10^{-21}$	
(32)	$HO_2 + NO \longrightarrow OH + NO_2$	3.5×10^{-12} exp (25	
(33)	$HO_2 + NO_2 \xrightarrow{M} HNO_4$	F(1.8(-31), 3.2, 4.7	
(34)	$HO_2 + NO_3 \longrightarrow HNO_3$	5.0×10^{-16}	
(35)	$HNO_4 \xrightarrow{M} HO_2 + NO_2$	$k_{33} \times 4.76 \times 10^{26}$ e	
(36)	$NO_3 + NO \longrightarrow 2NO_2$	1.5×10^{-11} exp (17	
(37)	$NO_3 + NO_2 \longrightarrow NO + NO_2$	4.5×10^{-14} exp (−	
(38)	$NO_3 + NO_2 \xrightarrow{M} N_2O_5$	F(2.2(-30), 3.9, 1.5	
(39)	$NO_3 + NO_3 \longrightarrow 2NO_2 + O_2$	8.5×10^{-13} exp (−	
(40)	$NO_3 + HO_2 \longrightarrow .3HNO_3 + .7NO_2 + .7OH$	3.5×10^{-12}	
(41)	$N_2O_5 + H_2O \longrightarrow 2HNO_3$	2.0×10^{-21}	
(42)	$N_2O_5 \xrightarrow{M} NO_3 + NO_2$	$k_{38} \times 3.7 \times 10^{26}$ e	
(43)	$NO + NO + O_2 \xrightarrow{O_2} 2NO_2$	3.3×10^{-39} exp (53	
(44)	$CO + OH \xrightarrow{O_2} HO_2$	$1.5 \times 10^{-13}(1 + .6$	
(45)	$SO_2 + OH \longrightarrow H_2SO_4 + HO_2$	F(3.0(-31), 3.3, 1.5	
	Paraffin Chemistry		
(46)	$CH_4 + OH \xrightarrow{O_2} CH_3O_2$	$T^{0.667} 2.8 \times 10^{-14}$	
(47)	$C_2H_6 + OH \longrightarrow ETHP$	$T^2 1.5 \times 10^{-17}$ exp	
(48)	$PAR + OH \longrightarrow RO_2$	8.1×10^{-13}	
(49)	$CH_3OH + OH \longrightarrow HCHO + HO_2$	6.7×10^{-12} exp (−	

Reaction Number	Reaction	Rate Constant, $k^{\dagger}$	Note
	Carbonyl Chemistry		
(50)	$HCHO + h\nu \xrightarrow{O_2} 2HO_2 + CO$	J_{HCHOa}	13,18
(51)	$HCHO + h\nu \longrightarrow CO$	J_{HCHOb}	13,18
(52)	$HCHO + OH \xrightarrow{O_2} HO_2 + CO$	1.0×10^{-11}	
(53)	$HCHO + NO_3 \xrightarrow{O_2} HNO_3 + HO_2 + CO$	3.4×10^{-13} exp (−	
(54)	$ALD2 + h\nu \xrightarrow{2O_2} CH_3O_2 + HO_2 + CO$	J_{ALD2}	
(55)	$ALD2 + OH \longrightarrow C_2O_3$	5.6×10^{-12} exp (2	
(56)	$ALD2 + NO_3 \xrightarrow{O_2} C_2O_3 + HNO_3$	1.4×10^{-12} exp (−	
(57)	$AONE + h\nu \xrightarrow{2O_2} C_2O_3 + CH_3O_2$	J_{AONE}	
(58)	$AONE + OH \longrightarrow ANO2$	$T^2 5.3 \times 10^{-18}$ exp	
(59)	$MGLY + h\nu \longrightarrow C_2O_3 + CO + HO_2$	$9.64 \times J_{HCHOa}$	
(60)	$MGLY + OH \longrightarrow XO_2 + C_2O_3$	1.7×10^{-11}	
(61)	$MGLY + NO_3 \longrightarrow HNO_3 + C_2O_3 + CO$	1.4×10^{-12} exp (−	
	Olefin chemistry		
(62)	$ETH + O_3 \longrightarrow HCHO + 0.22HO_2 + 0.12OH + 0.24CO + 0.24CO_2 + 0.52HCOOH$	1.2×10^{-14} exp (−	
(63)	$ETH + OH \longrightarrow XO_2 + 1.56HCHO + HO_2 + 0.22ALD2$	F(1.0(-28), 0.8, 8.8	
(64)	$OLET + O_3 \longrightarrow 0.57HCHO + 0.47ALD2 + 0.33OH + 0.26HO_2 + 0.08H_2 + 0.07CH_3O_2 + 0.06ETHP + 0.03RO_2 + 0.13C_2O_3 + 0.04MGLY + 0.03CH_3OH + 0.06CH_4 + 0.01C_2H_6 + 0.31CO + 0.22CO_2 + 0.22HCOOH + 0.09RCOOH - 1.06PAR$	4.2×10^{-15} exp (−	
(65)	$OLEI + O_3 \longrightarrow 1.03ALD2 + 0.07AONE + 0.60OH + 0.22HO_2 + 0.10CH_3O_2 + 0.05ETHP + 0.09RO_2 + 0.14ANO_2 + 0.19C_2O_3 + 0.07MGLY + 0.04CH_3OH + 0.08CH_4 + 0.01C_2H_6 + 0.30CO + 0.18CO_2 + 0.16RCOOH - 2.26PAR$	8.9×10^{-16} exp (−	
(66)	$OLET + OH \longrightarrow XO_2 + HO_2 + HCHO + ALD2 - PAR$	5.8×10^{-12} exp (4	
(67)	$OLEI + OH \longrightarrow XO_2 + HO_2 + 0.23AONE + 1.77ALD2 - 2.23PAR$	2.9×10^{-11} exp (2	
(68)	$OLET + NO_3 \longrightarrow NAP$	3.1×10^{-13} exp (−	
(69)	$OLEI + NO_3 \longrightarrow NAP$	2.5×10^{-12}	
	Aromatic Chemistry		
(70)	$TOL + OH \longrightarrow 0.08XO_2 + 0.2HO_2 + 0.12CRES + 0.8TO_2$	2.1×10^{-12} exp (3	
(71)	$XYL + OH \longrightarrow 0.5XO_2 + 0.55HO_2 + 0.8MGLY + 1.1PAR + 0.45TO_2 + 0.05CRES$	1.7×10^{-11} exp (1	
(72)	$TO_2 + NO \longrightarrow 0.95(NO_2 + OPEN + HO_2) + 0.05ONIT$	8.1×10^{-12}	
(73)	$CRES + OH \longrightarrow 0.4CRO + 0.6XO_2 + 0.6HO_2 + 0.3OPEN$	4.1×10^{-11}	
(74)	$CRES + NO_3 \longrightarrow CRO + HNO_3$	2.2×10^{-11}	
(75)	$CRO + NO_2 \longrightarrow ONIT$	1.4×10^{-11}	
(76)	$OPEN + OH \longrightarrow XO_2 + C_2O_3 + 2CO + 2HO_2 + HCHO$	3.0×10^{-11}	
(77)	$OPEN + h\nu \longrightarrow C_2O_3 + CO + HO_2$	$9.04 \times J_{HCHOa}$	
(78)	$OPEN + O_3 \longrightarrow 0.03ALD2 + 0.62C_2O_3 + 0.7HCHO + 0.69CO + 0.08OH + 0.03XO_2 + 0.76HO_2 + 0.2MGLY$	5.4×10^{-17} exp (−	
	Isoprene Chemistry		
(79)	$ISOP + OH \longrightarrow ISOPP + 0.08XO2$	2.55×10^{-11} exp (	
(80)	$ISOP + O_3 \longrightarrow 0.6HCHO + 0.65ISOPRD + 0.27OH + 0.07CO + 0.39RCOOH + 0.07HO_2 + 0.15ALD2 + 0.2XO_2 + 0.2C_2O_3$	1.2×10^{-14} exp (	
(81)	$ISOP + NO_3 \longrightarrow ISOPN$	3.0×10^{-12} exp (−	
(82)	$ISOPRD + OH \longrightarrow 0.5C_2O_3 + 0.5ISOPO_2 + 0.2XO_2$	3.3×10^{-11}	
(83)	$ISOPRD + O_3 \longrightarrow 0.27OH + 0.1HO_2 + 0.11C_2O_3 + 0.07XO_2 + 0.05CH_3O_2 + 0.16CO + 0.15HCHO + 0.02ALD + 0.09AONE + 0.85MGLY + 0.46RCOOH$	7.0×10^{-18}	
(84)	$ISOPRD + h\nu \longrightarrow 0.97C_2O_3 + 0.33HO_2 + 0.33CO + 0.7CH_3O_2 + 0.2HCHO + 0.07ALD + 0.03AONE$	J_{ISOPRD}	
(85)	$ISOPRD + NO_3 \longrightarrow 0.07C_2O_3 + 0.07HNO_3 + 0.64CO + 0.28HCHO + 0.93ONIT + 0.28ALD2 + 0.93HO_2 + 0.93XO_2 + 1.86PAR$	1.0×10^{-15}	

Reaction Number	Reaction	Rate Constant, $k^{\dagger}$	Note
	Organic Hydroperoxides		
(86)	$CH_3OOH + h\nu \xrightarrow{O_2} HCHO + HO_2 + OH$	J_{CH_3OOH}	11,18
(87)	$ETHOOH + h\nu \longrightarrow ALD2 + HO_2 + OH$	same as reaction (86)	9,11
(88)	$ROOH + h\nu \longrightarrow OH + 0.4XO_2 + 0.74AONE + 0.3ALD2 + 0.1ETHP + 0.9HO_2 - 1.98PAR$	same as reaction (86)	9,11
(89)	$CH_3OOH + OH \longrightarrow 0.7CH_3O_2 + 0.3HCHO + 0.3OH$	3.8×10^{-12} exp $(200/T)$	1,11
(90)	$ETHOOH + OH \longrightarrow 0.7ETHP + 0.3ALD2 + 0.3OH$	3.8×10^{-12} exp $(200/T)$	9,11
(91)	$ROOH + OH \longrightarrow 0.77RO_2 + 0.19MGLY + 0.04ALD2 + 0.23OH \; 0.12PAR$	3.8×10^{-12} exp $(200/T)$	9,11
	Organic Nitrates		
(92)	$ONIT + OH \longrightarrow NAP$	1.6×10^{-11} exp $(-540/T)$	11,12
(93)	$ONIT + h\nu \longrightarrow NO_2 + 0.41XO_2 + 0.74AONE + 0.3ALD2 + 0.1ETHP + 0.9HO_2 - 1.98PAR$	J_{ONIT}	11,18
(94)	$C_2O_3 + NO_2 \longrightarrow PAN$	F(9.7(-29), 5.6, 9.3(-12), 1.5)	1,13
(95)	$PAN \longrightarrow C_2O_3 + NO_2$	$k_{94} 1.1 \times 10^{28}$ exp $(-14000/T)$	1,13
	Alkyl and Acyl Peroxy Radical Chemistry		
(96)	$CH_3O_2 + NO \longrightarrow HCHO + HO_2 + NO_2$	3.0×10^{-12} exp $(280/T)$	1,11
(97)	$ETHP + NO \longrightarrow ALD2 + HO_2 + NO_2$	2.6×10^{-12} exp $(365/T)$	1,11
(98)	$RO_2 + NO \longrightarrow 0.16ONIT + 0.84NO_2 + 0.34XO_2 + 0.62AONE + 0.25ALD2 + 0.08ETHP + 0.76HO_2 - 1.68PAR$	4.0×10^{-12}	8,11
(99)	$C_2O_3 + NO \xrightarrow{O_2} CH_3O_2 + NO_2 + CO_2$	5.3×10^{-12} exp $(360/T)$	1,10
(100)	$ANO2 + NO \longrightarrow NO_2 + C_2O_3 + HCHO$	4.0×10^{-12}	8,11
(101)	$NAP + NO \longrightarrow 1.5NO_2 + 0.5HCHO + 0.5ALD2 + 0.5ONIT + 0.5HO_2 - PAR$	4.0×10^{-12}	8,11
(102)	$ISOPP + NO \longrightarrow 0.09ONIT + 0.91NO_2 + 0.91HO_2 + 0.63HCHO + 0.91ISOPRD + 0.18PAR$	4.0×10^{-12}	8,15
(103)	$ISOPN + NO \longrightarrow NO_2 + 0.8ALD2 + 0.8ONIT + 0.8HO_2 + 0.2ISOPRD + 0.2NO_2 + 1.6PAR$	4.0×10^{-12}	8,15
(104)	$ISOPO_2 + NO \longrightarrow NO_2 + HO_2 + 0.59CO + 0.55ALD2 + 0.25HCHO + 0.34MGLY + 0.63AONE$	4.0×10^{-12}	8,15
(105)	$XO_2 + NO \longrightarrow NO_2$	4.0×10^{-12}	8,13
(106)	$CH_3O_2 + NO_3 \longrightarrow HCHO + HO_2 + NO_2$	1.1×10^{-12}	7,11
(107)	$ETHP + NO_3 \longrightarrow ALD2 + HO_2 + NO_2$	2.5×10^{-12}	7,11
(108)	$RO_2 + NO_3 \longrightarrow NO_2 + 0.4XO_2 + 0.74AONE + 0.3ALD2 + 0.1ETHP + 0.9HO_2 - 1.98PAR$	2.5×10^{-12}	7,11
(109)	$C_2O_3 + NO_3 \longrightarrow CH_3O_2 + NO_2$	4.0×10^{-12}	8,11
(110)	$ANO2 + NO_3 \longrightarrow NO_2 + C_2O_3 + HCHO$	1.2×10^{-12}	8,11
(111)	$NAP + NO_3 \longrightarrow 1.5NO_2 + 0.5HCHO + 0.5ALD2 + 0.5ONIT + 0.5HO_2 - PAR$	4.0×10^{-12}	8,11
(112)	$XO_2 + NO_3 \longrightarrow NO_2$	2.5×10^{-12}	7,11
(113)	$CH_3O_2 + HO_2 \longrightarrow CH_3OOH$	3.8×10^{-13} exp $(800/T)$	1,11
(114)	$ETHP + HO_2 \longrightarrow ETHOOH$	7.5×10^{-13} exp $(700/T)$	1,11
(115)	$RO_2 + HO_2 \longrightarrow ROOH$	1.7×10^{-13} exp $(1300/T)$	8,11
(116)	$C_2O_3 + HO_2 \longrightarrow 0.4(RCOOH + O_3)$	4.5×10^{-13} exp $(1000/T)$	1,10
(117)	$ANO2 + HO_2 \longrightarrow ROOH$	1.2×10^{-13} exp $(1300/T)$	8,11
(118)	$NAP + HO_2 \longrightarrow ONIT$	1.7×10^{-13} exp $(1300/T)$	8,11
(119)	$ISOPP + HO_2 \longrightarrow ROOH$	1.7×10^{-13} exp $(1300/T)$	8,15
(120)	$ISOPN + HO_2 \longrightarrow ONIT + 2PAR$	1.7×10^{-13} exp $(1300/T)$	8,15
(121)	$ISOPO_2 + HO_2 \longrightarrow ROOH$	1.7×10^{-13} exp $(1300/T)$	8,15
(122)	$XO_2 + HO_2 \longrightarrow$	1.7×10^{-13} exp $(1300/T)$	8,11
	Parameterized Permutation Reactions		
(123)	$CH_3O_2 \longrightarrow 0.66HCHO + 0.32HO_2 + 0.34CH_3OH$	$k_i^{(1)}, i = CH_3O_2$	11,16
(124)	$ETHP \longrightarrow 0.8ALD2 + 0.6HO_2 + 0.2C_2H_6$	$k_i^{(1)}, i = ETHP$	11,16
(125)	$RO_2 \longrightarrow 0.24XO_2 + 0.21ALD2 + 0.57AONE + 0.06ETHP + 0.54HO_2 - 1.25PAR$	$k_i^{(1)}, i = RO_2$	11,16 11,16
(126)	$C_2O_3 \longrightarrow CH_3O_2 + CO_2$	$k_i^{(1)}, i = C_2O_3$	11,16
(127)	$ANO2 \longrightarrow 0.7(C_2O_3 + HCHO) + 0.15(MGLY + AONE)$	$k_i^{(1)}, i = ANO2$	11,16
(128)	$NAP \longrightarrow 0.5(NO_2 + HCHO + ALD2 + ONIT) - PAR$	$k_i^{(1)}, i = NAP$	11,16

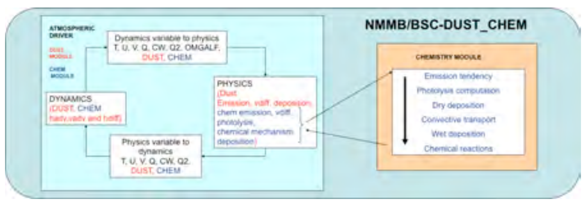
NMMB/BSC-Chemical Transport Model (Overview)

- fully on-line access coupling: feedback processes allowed
- multiscale: global to regional scales allowed

NMMB/ BSC-CTM

Nonhydrostatic Multiscale Model on the B-grid (NMMB)
meteo variables/parameters

→ *Janjic and Gall (NCAR/TN 2012)*
→ *Janjic and Vasic (EGU2012)*
→ *Janjic et al. (MWR 2011)*
→ *(...)*

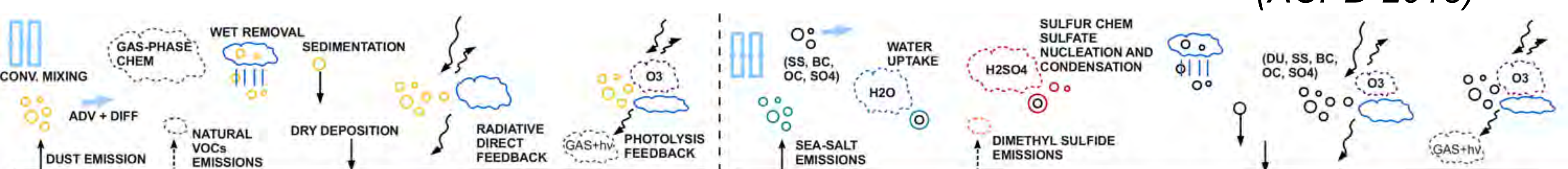


BSC Chemical Transport Model
(gas/aerosol variables: mass mixing ratios)

GAS-PHASE CHEM (52 species) → *Jorba et al. (JGR 2012)*

DUST (8 bins) → *Pérez et al. (ACP 2011)* → *Haustein et al. (ACP 2012)*

SEA-SALT → *Spada et al. (ACPD 2013)*



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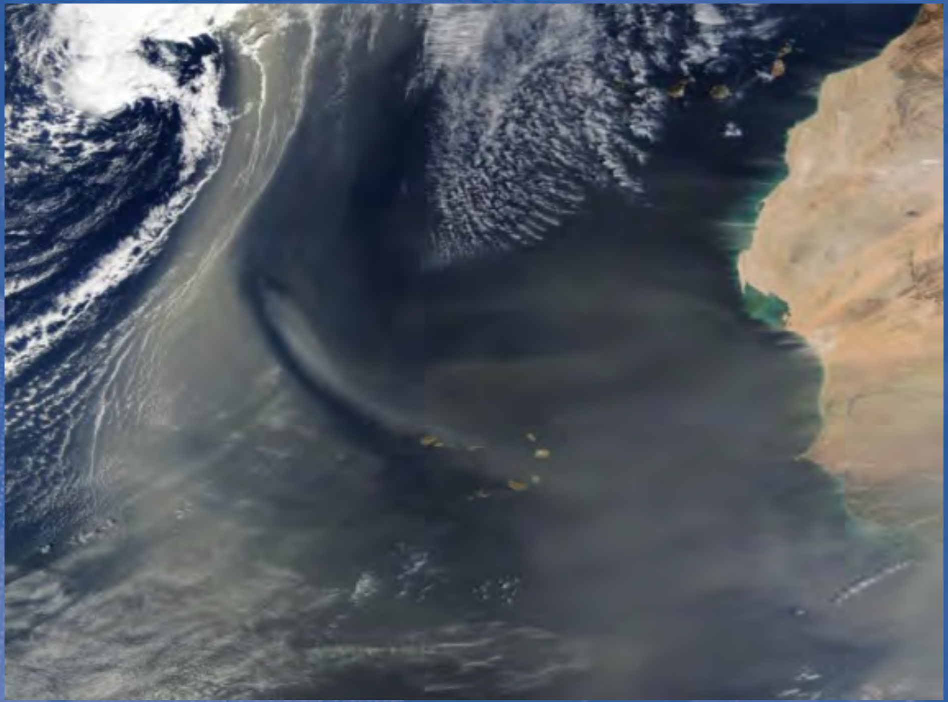
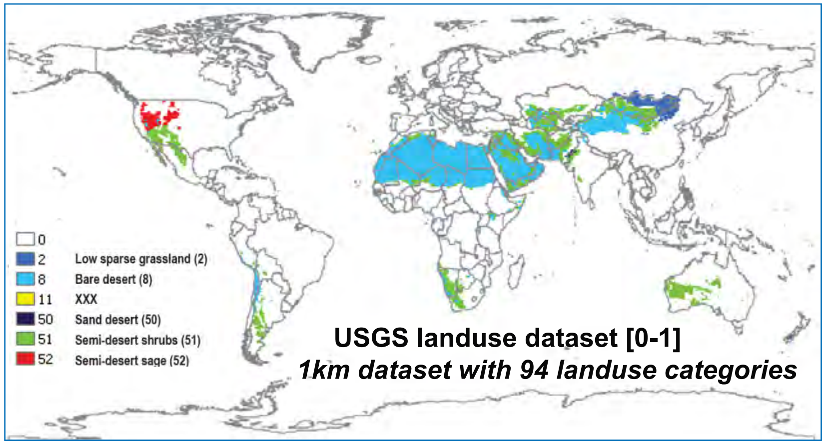
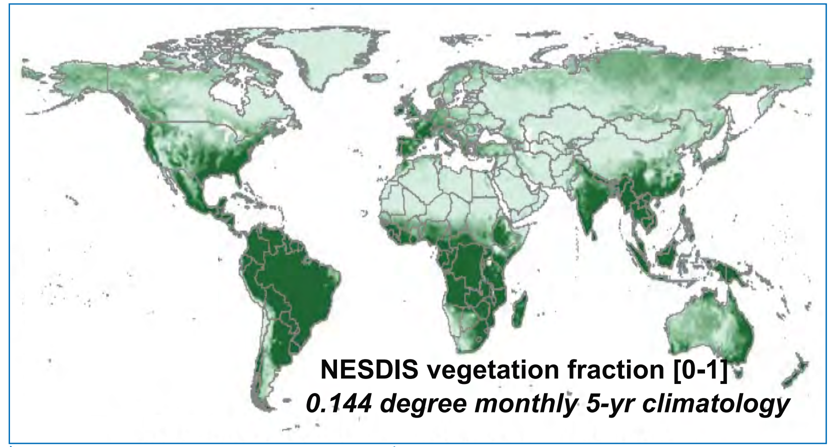


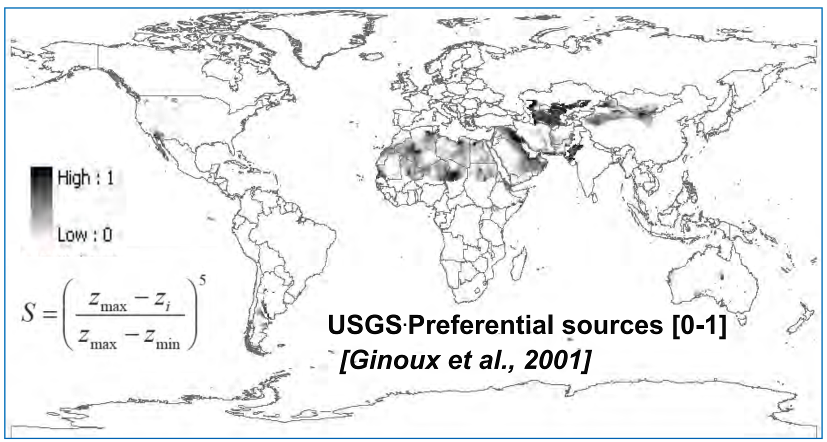
MINERAL DUST MODULE

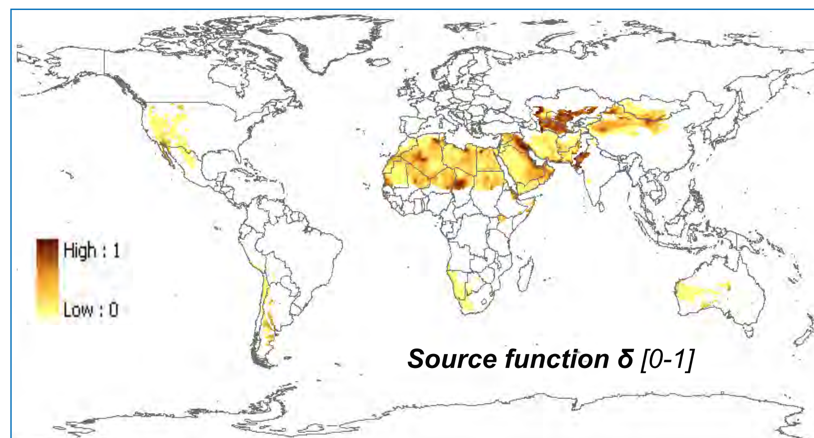
The NMMB/BSC-DUST model (Pérez et al., 2011)

Source function: update databases









$$\delta = USGS \cdot PREF \cdot (1 - VEGFRAC) \cdot (1 - SnowCover)$$

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The NMMB/BSC-DUST: Regional domain

Satellite comparison for 2006 (Pérez et al., 2011)

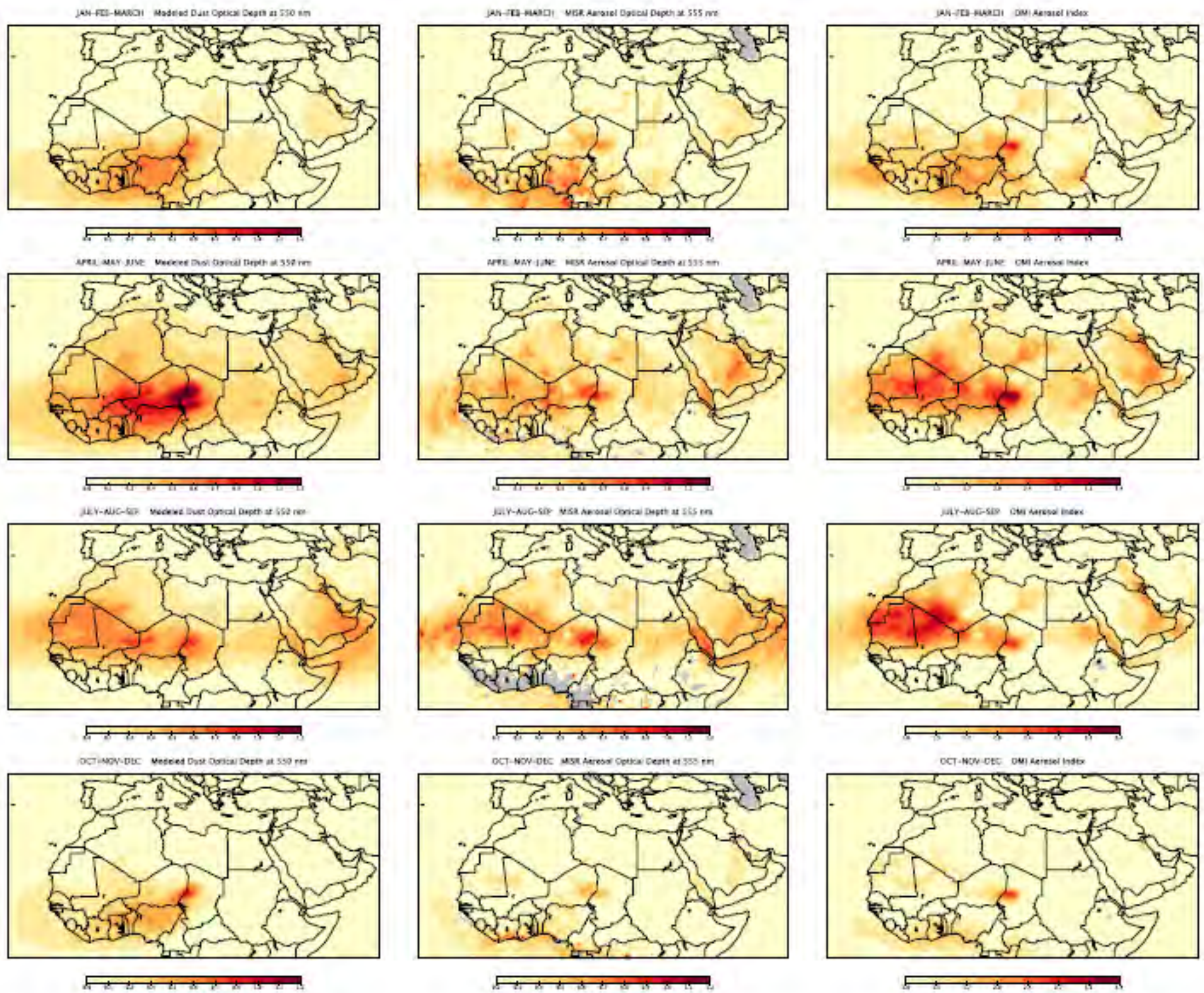
NMMB/BSC-DUST | MISR | OMI

Winter

Spring

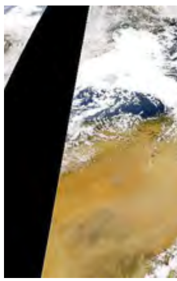
Summer

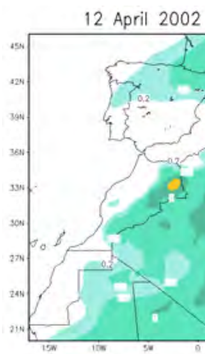
Autumn

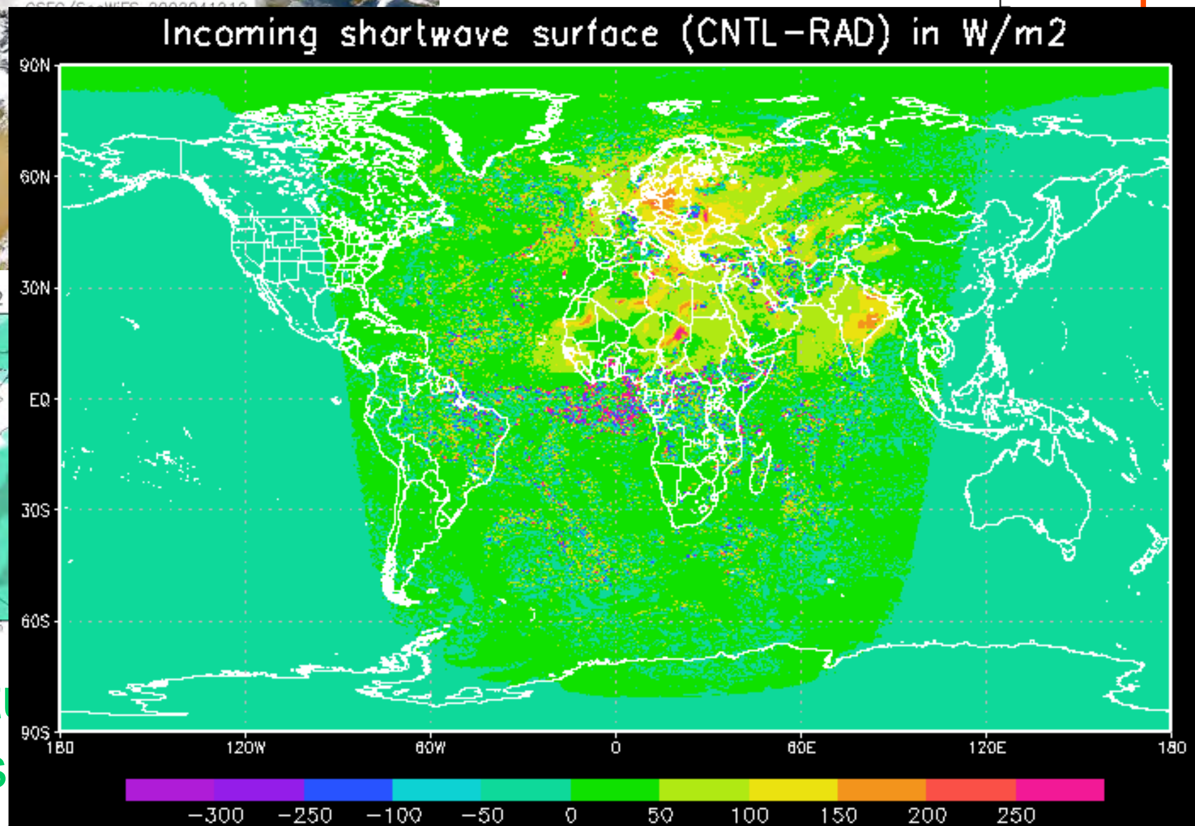


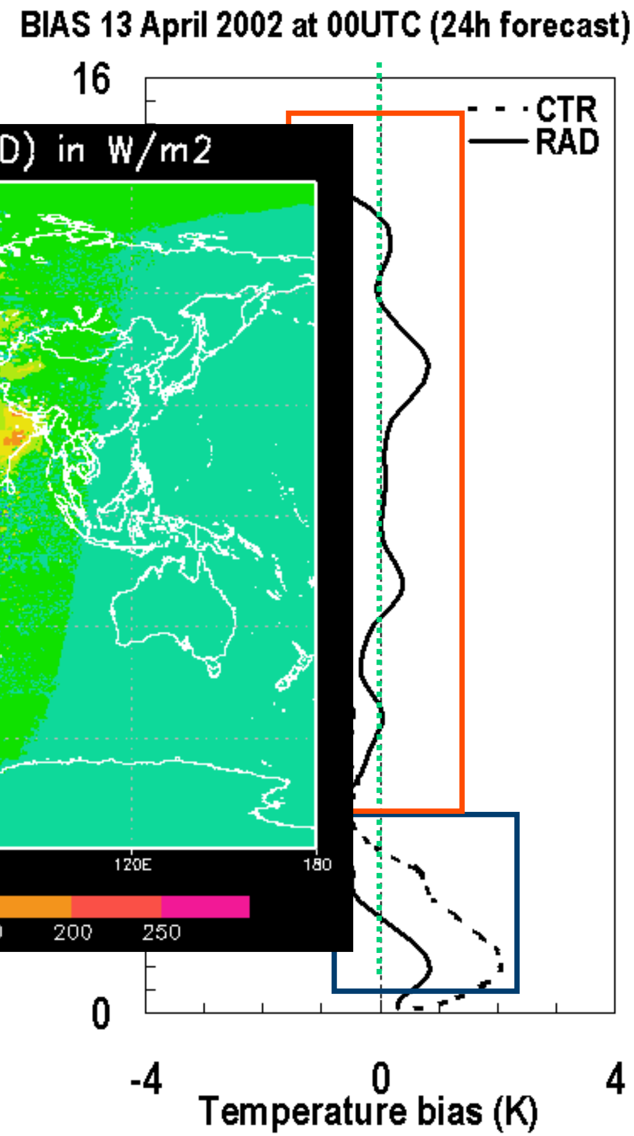
Feedbacks: Dust-radiation interaction

Improvements in NWP





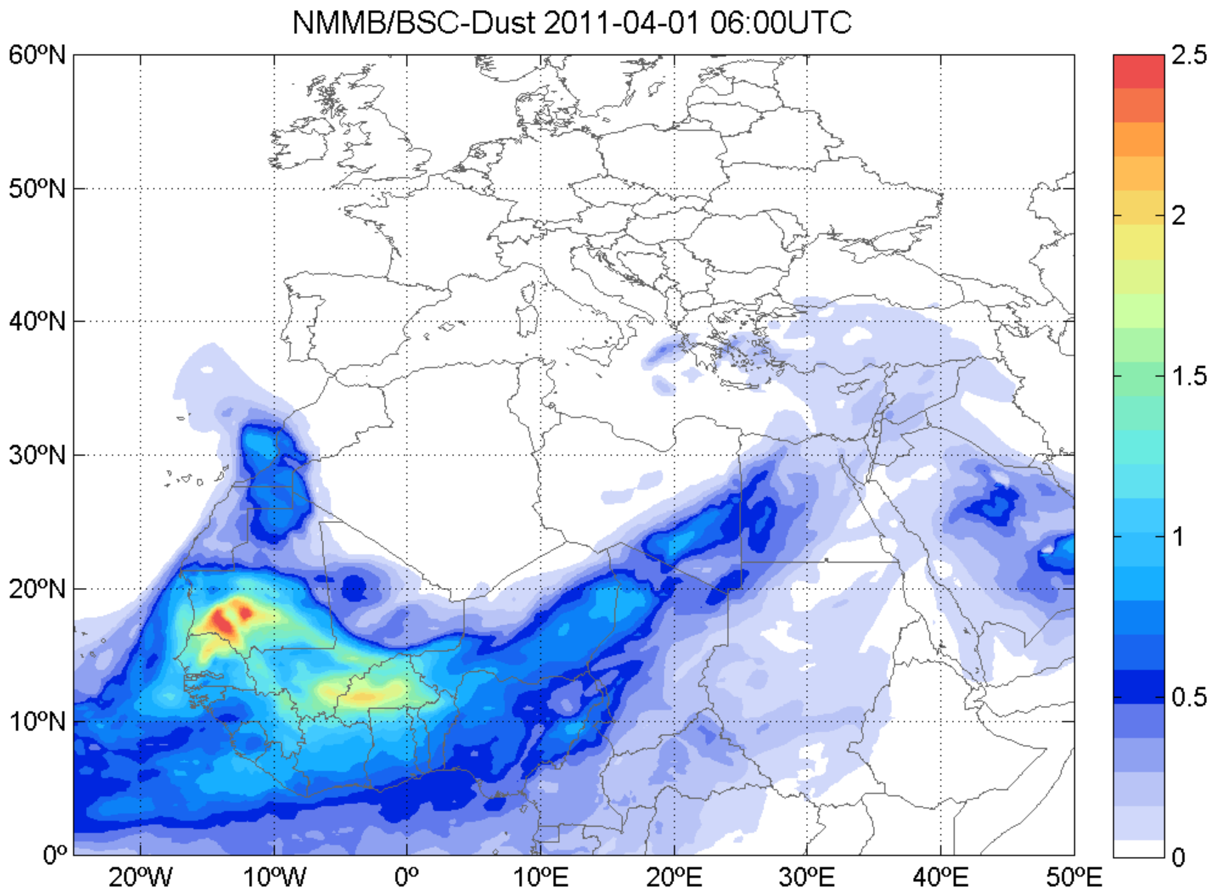




- ✓ Pert
  mos
- ✓ Reduction of the low level warm bias
  - ✓ Reduction of the upper level cold bias

(Pérez et al., 2006; Pérez et al., 2011)

Dust AOD at 550nm April 2011



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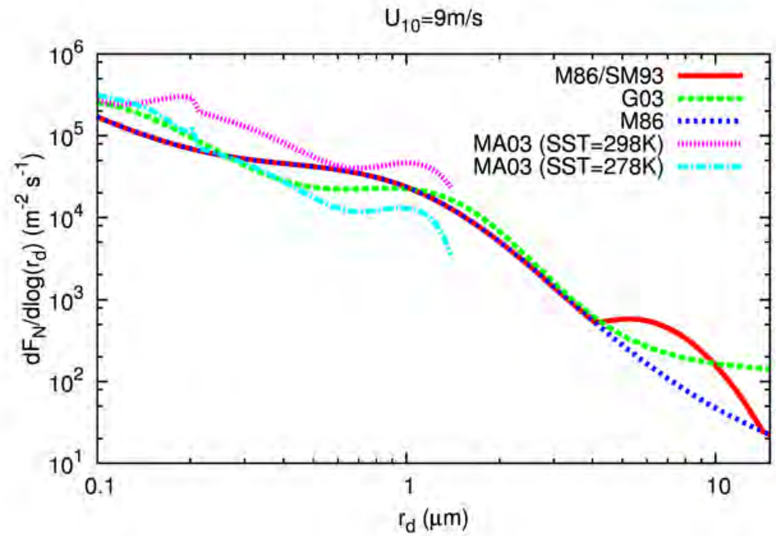
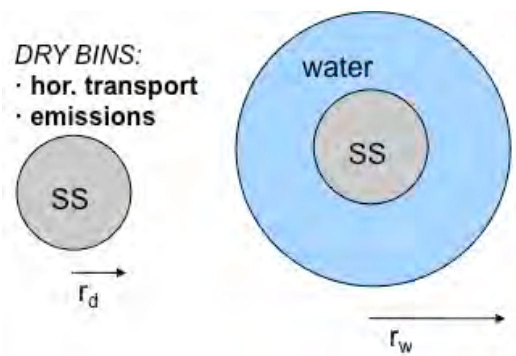
SEA SALT AEROSOL MODULE

The sea-salt module (Spada et al., 2013)

→ emission of ssa aerosol depends on surface wind speed and SST



→ aerosol module extended to wet aerosol

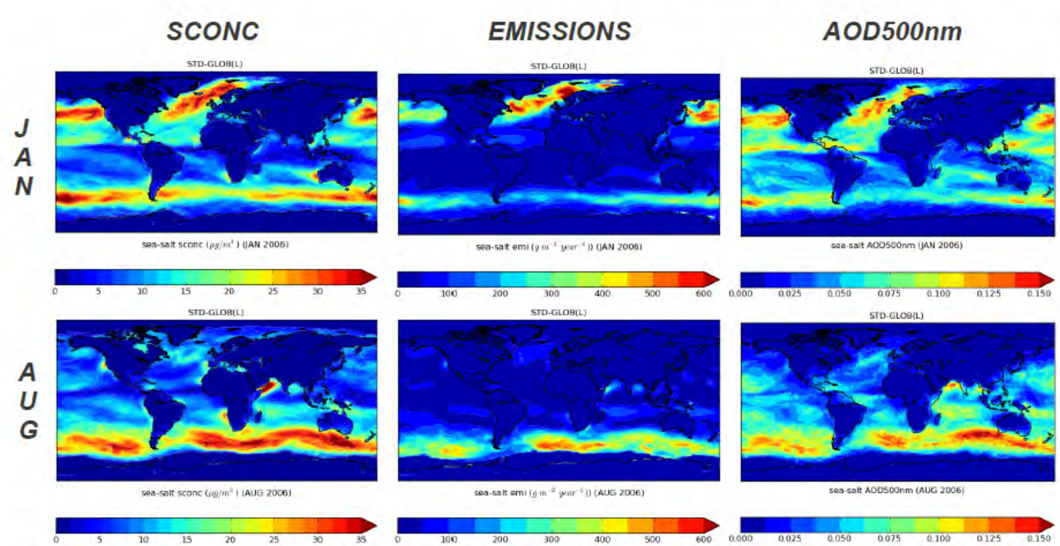


→ NMMB/BSC-CTM, ref year 2006
· emi total: 7307.8 Tg/y
· load: 6.6 Tg
· lifetime 9.56h

– AEROCOM median, year 2000
· emi total: 6212.3 Tg/y
· load: 6.1 Tg
· lifetime 8.64h

$$r_d \rightarrow r_w = r_d \cdot \Phi(RH)$$

$$\rho_d \rightarrow \rho_w = \rho_d \Phi^{-3} + (1-\Phi^{-3})\rho_{water}$$



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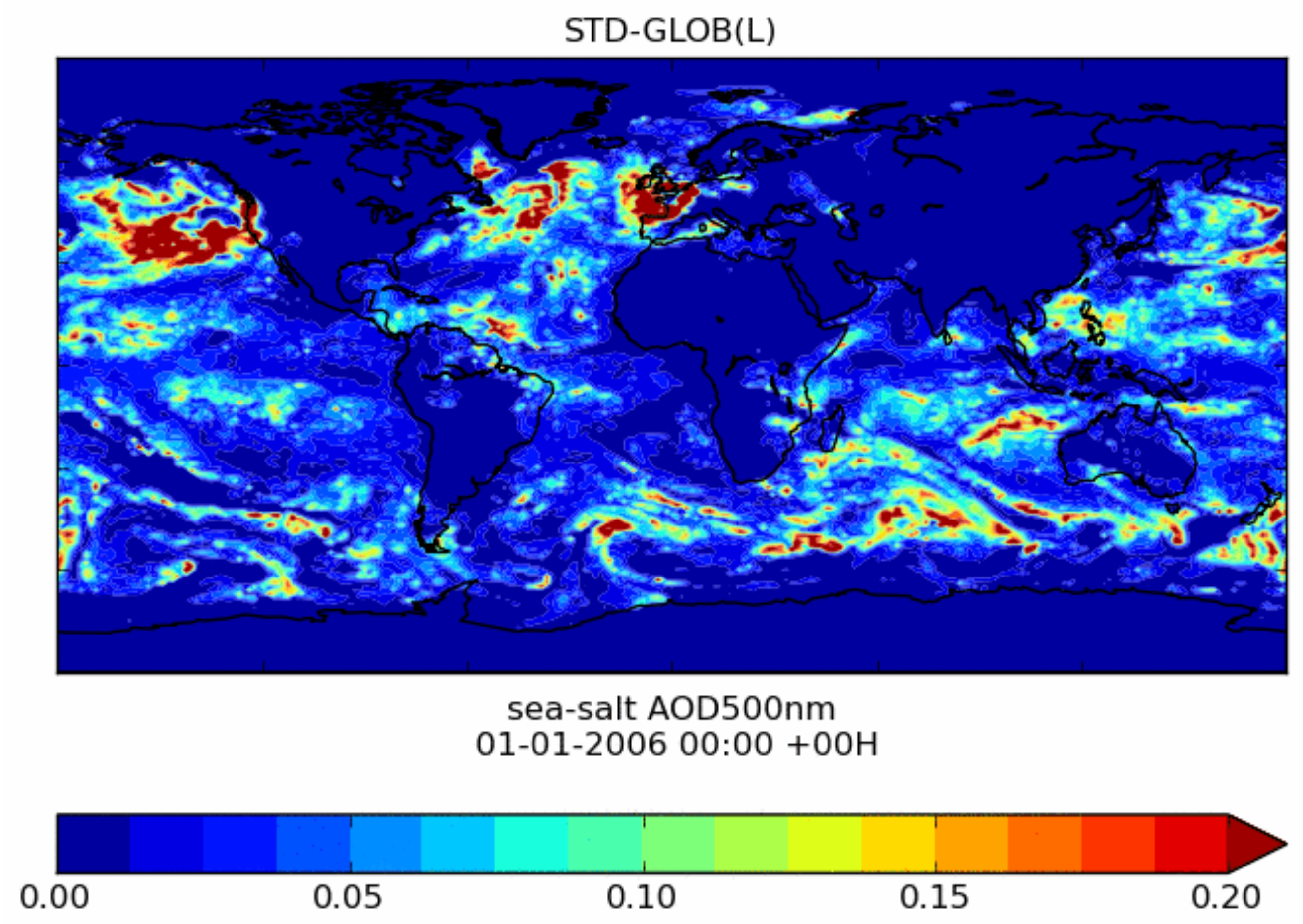
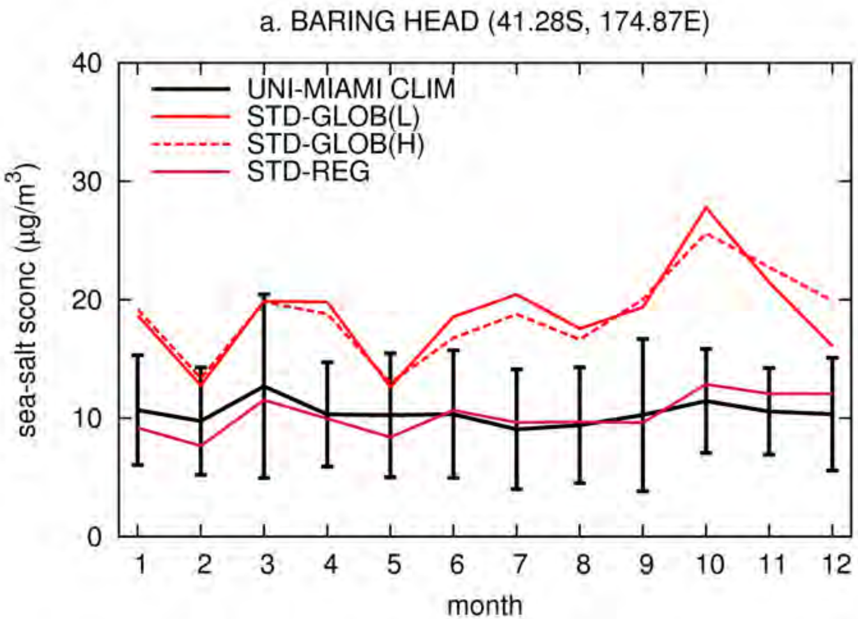
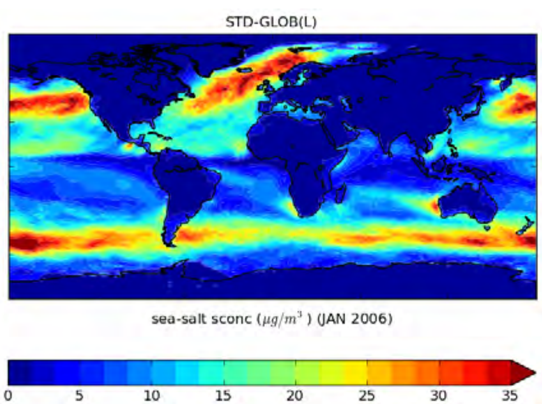
SEA-SALT AOD500nm

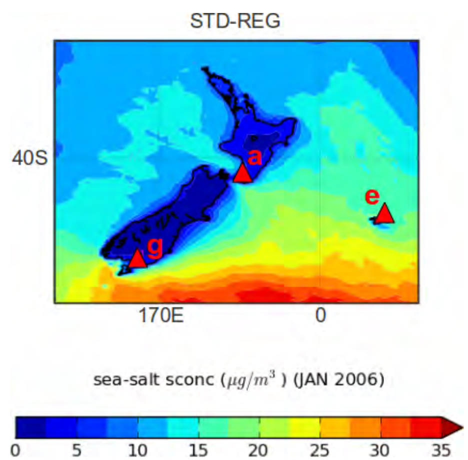


Impact of resolution

- GLOB(L) and GLOB(H) resolutions seem to give quite similar results, although...



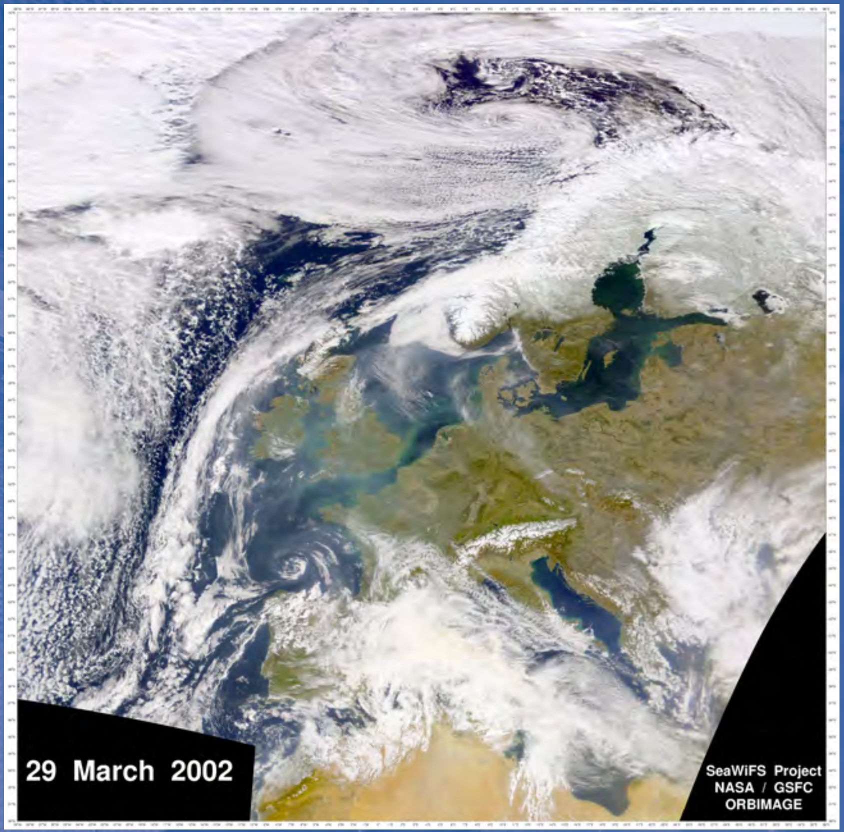




→ at smaller scales (REG = 0.1 x 0.1) the model becomes able to resolve steep topographies

→ in these cases (such as for the New Zealand domain), the observed SCONC climatologies are reproduced

→ obvious but not trivial: smaller scales (≈0.1deg) effects may affect larger scales (>1deg)



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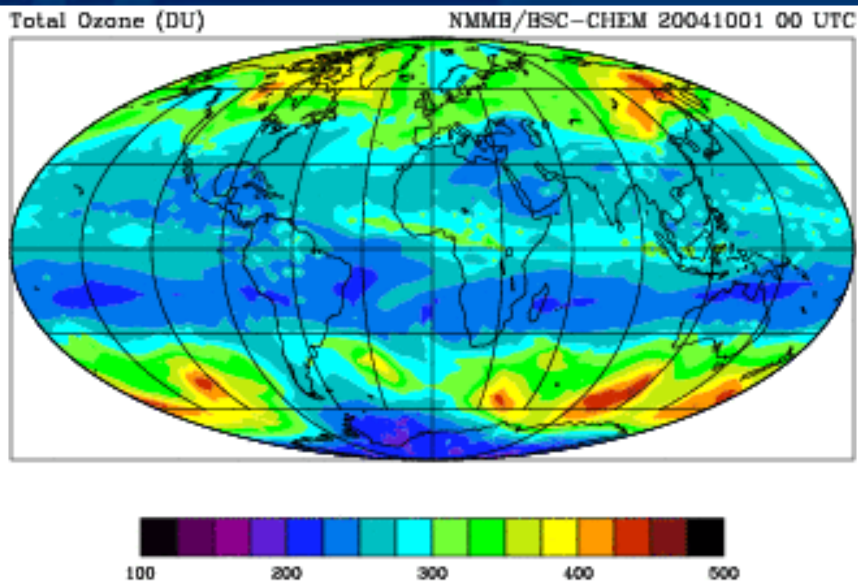
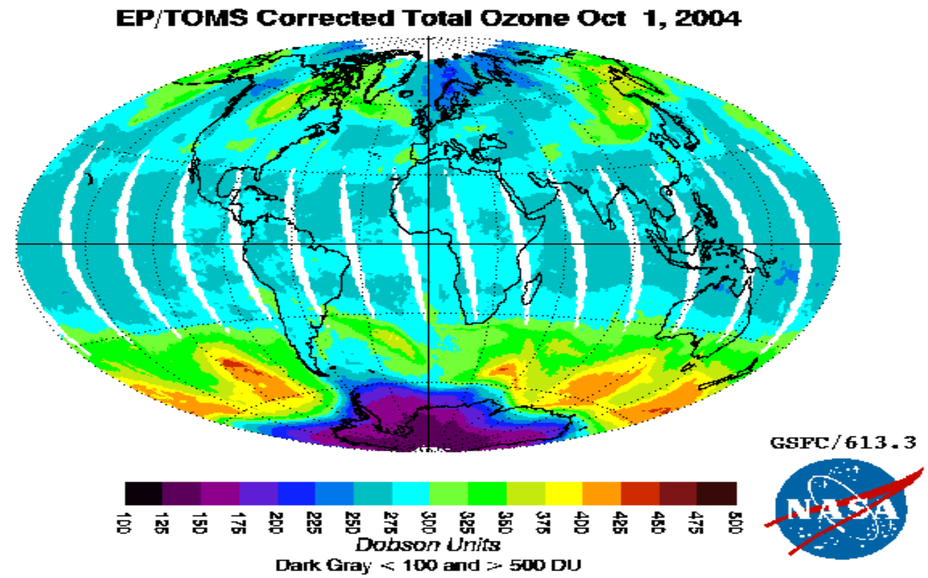
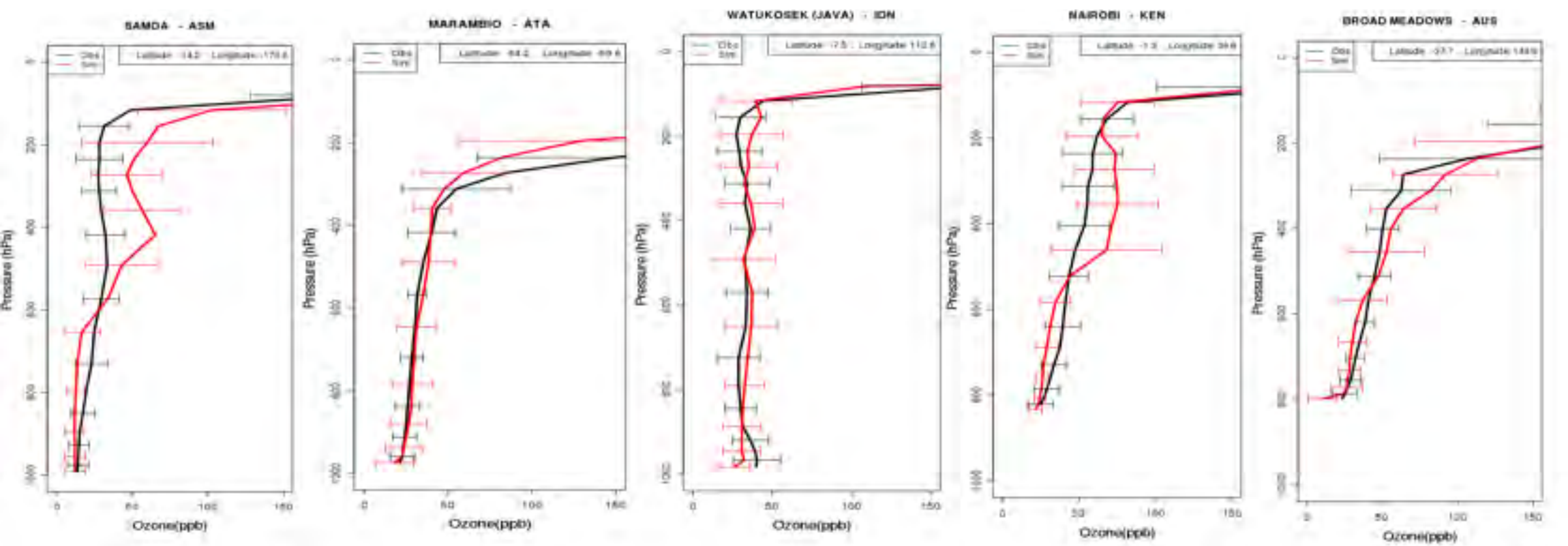
GAS-PHASE MODULE

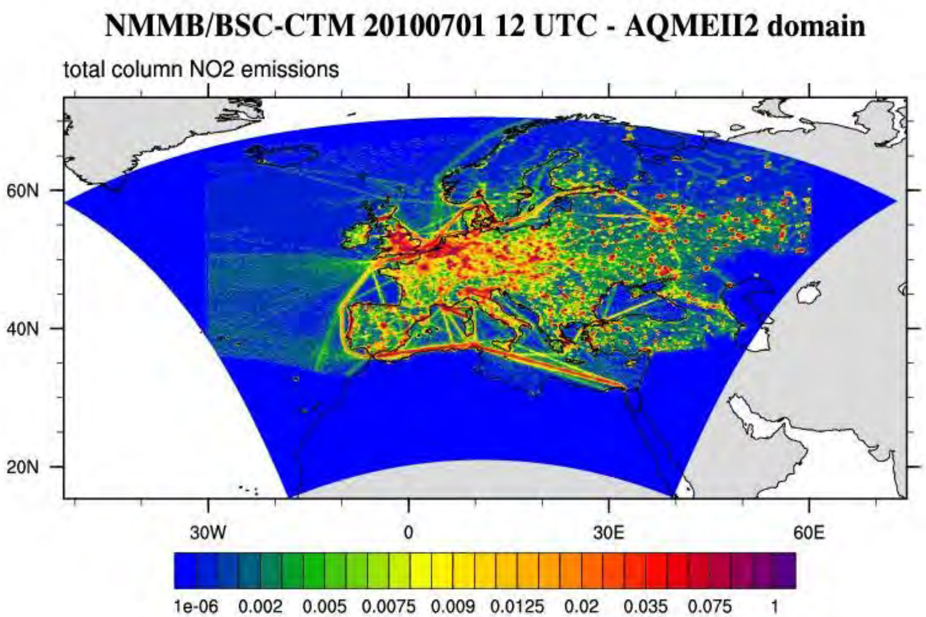
Gas phase results

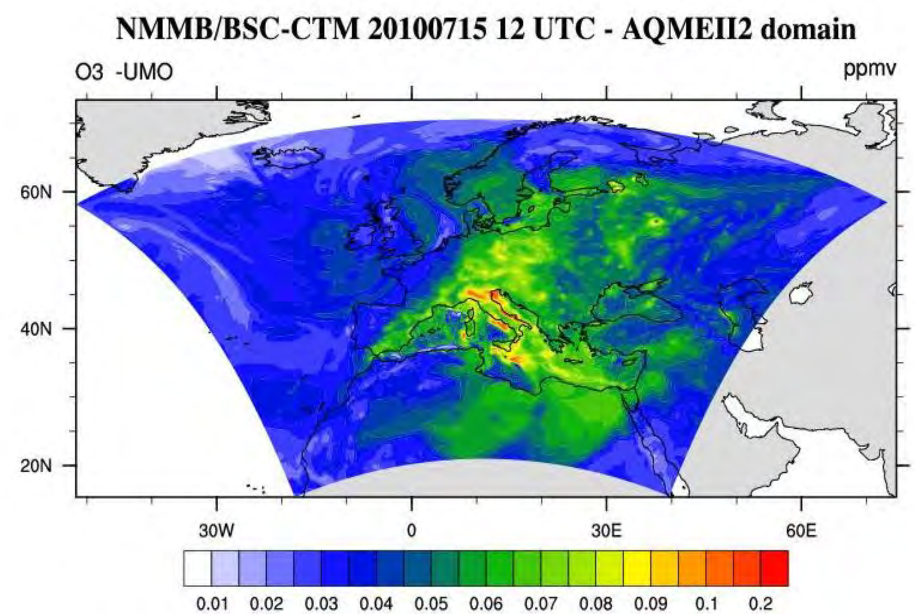


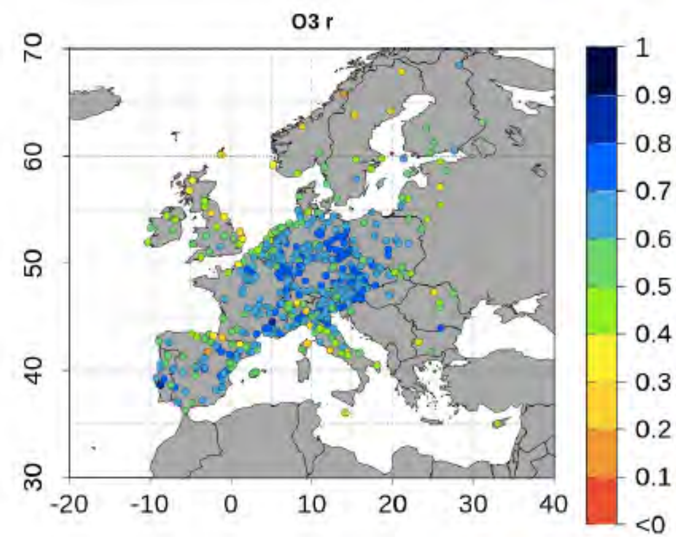


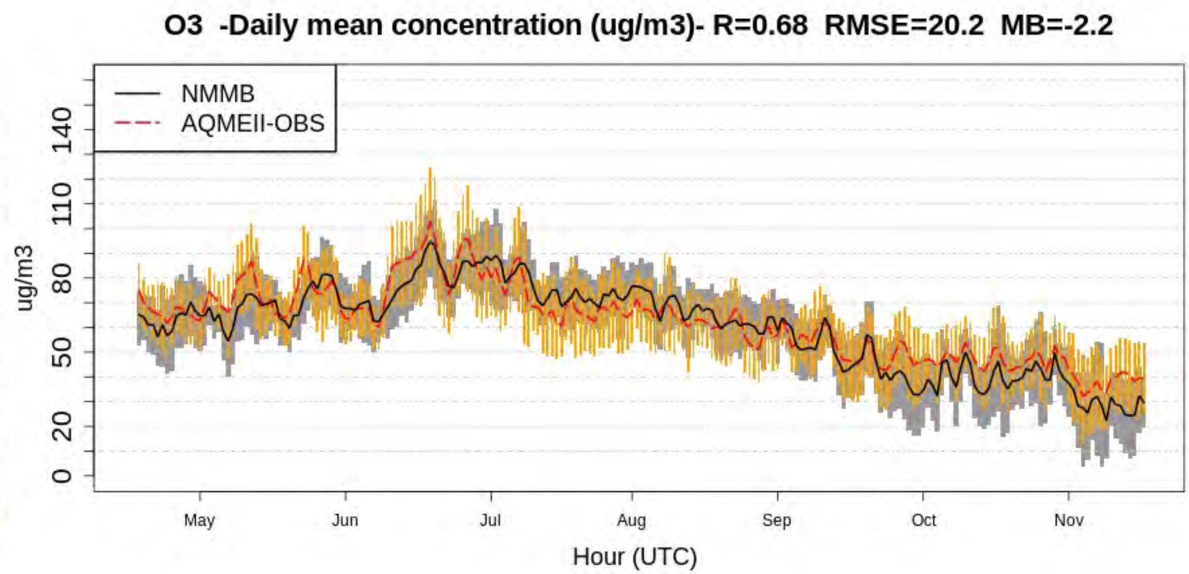


Regional run results

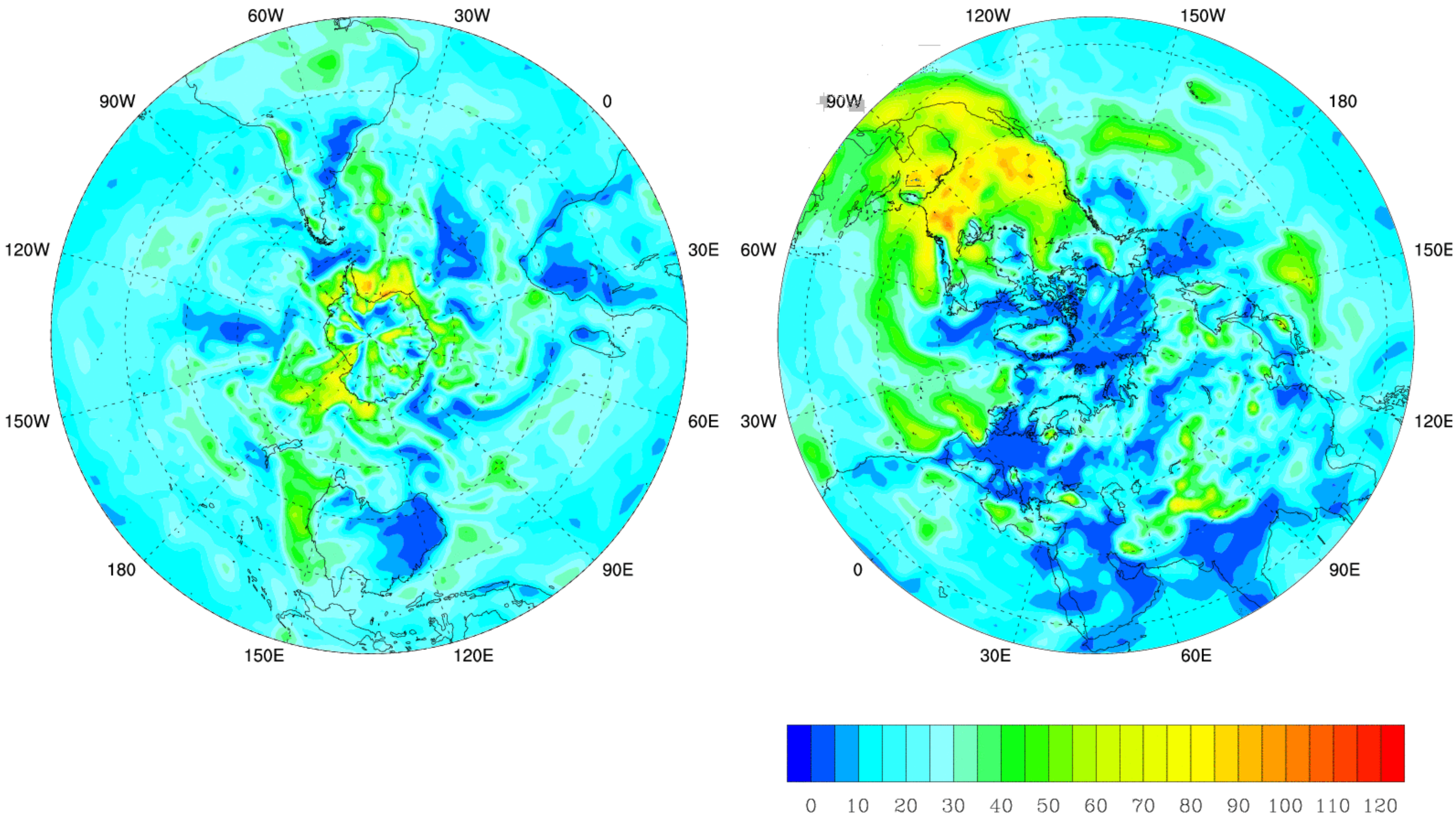








Ozone surface concentration in summer (ppb)



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FUTURE WORK

Future Developments

- Coupling of chemistry gas-phase with a secondary aerosol scheme for LAM applications at high-resolutions.
- Implementation of the other global relevant aerosol species, i.e. black (BC) and organic carbon (OC), and sulfate (SO4), in addition to dust (DU) and sea salt (SSA).
- Implementation of a volcanic ash module (Fall3D model, Folch et al., 2008) within the modeling system
- Implement effects of aerosols on meteorology
- Coupling the model with an ocean model for climate applications
- Explore methodologies for aerosol data assimilation

Providing forecast products for

· **Mineral dust forecasts for SDS-WAS North Africa, Middle East and Europe portal**

http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast

· **Participate in the ICAP global-model intercomparison project**

http://www.nrlmry.navy.mil/aerosol/icap.1087.php

· **Participate in the Charmex Chemistry-Aerosol Mediterranean experiment**

· **Participate in the AQMEII on-line Air Quality model intercomparison project** www.bsc.es

EXCELENCIA SEVERO OCHOA

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Thank you!

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