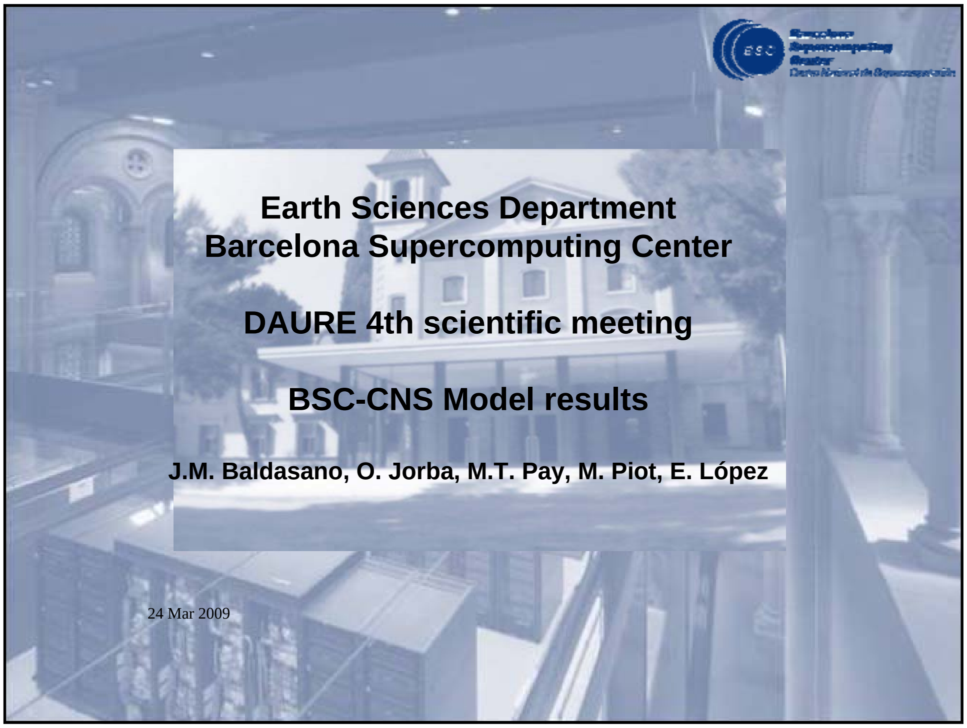


Earth Sciences Department
Barcelona Supercomputing Center

DAURE 4th scientific meeting

BSC-CNS Model results

J.M. Baldasano, O. Jorba, M.T. Pay, M. Piot, E. López

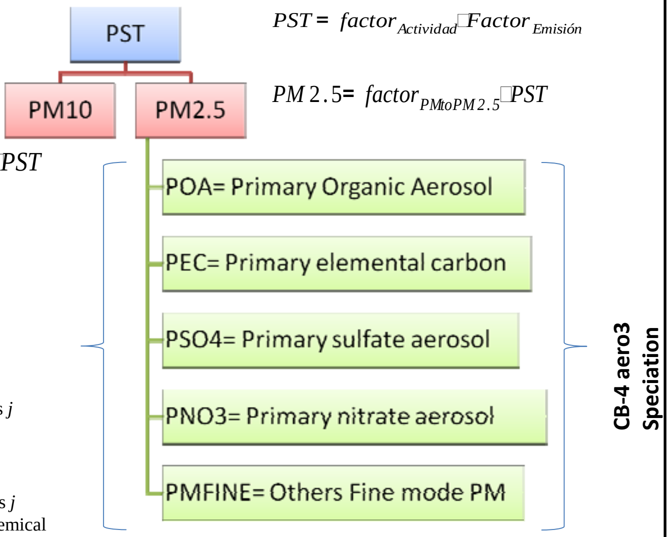
24 Mar 2009

How do we estimate PM Emissions

$$PST = factor_{Actividad} \cdot Factor_{Emisión}$$

$$PM2.5 = factor_{PMtoPM2.5} \cdot PST$$

$$PM10 = factor_{PMtoPM10} \cdot PST$$



PST

PM10

PM2.5

POA= Primary Organic Aerosol

PEC= Primary elemental carbon

PSO4= Primary sulfate aerosol

PNO3= Primary nitrate aerosol

PMFINE= Others Fine mode PM

CB-4 aero3 Speciation

$$E_j(k) = E(k) \cdot factor_j$$

$E_j(k)$:	PM2.5 emission for species j
$E(k)$:	$PM_{2.5}$ emission
$factor_j$:	speciation factor for species j following CB-4 – aero3 chemical mechanism

Example for Snap-07 sector : Road Transport

- Exhaust Emissions
  - Hot emissions
  - Cold start emissions

PM10= PM2.5 ⇨PMcoarse=PM10-PM2.5= 0

- Non-exhaust emissions
  - Particles from Tyre
  - Particles from Brake wear
  - Particles from road surface wear

PM2.5/PM10= 0.55

- PM2.5 Speciation

Species:	**POA**	**PEC**	**PSO_4**	**PNO_3**	**PMFINE**
$factor_j$	0.3637	0.6130	0.0044	0.0006	0.0183

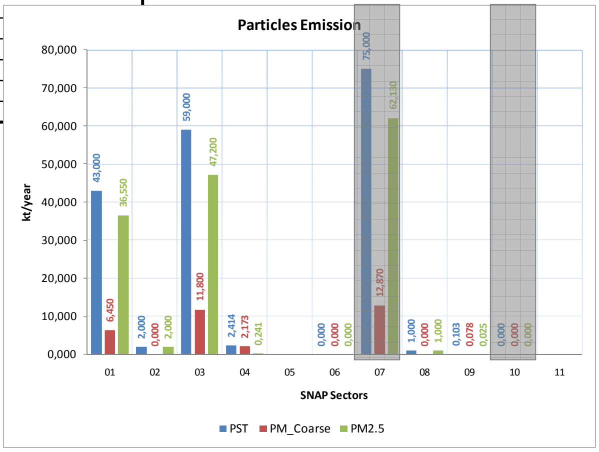
PM emission distribution by SNAP sectors

SNAP sector	Description
01	Combustion in energy and transformation industries
02	Non-industrial combustion plants
03	Combustion in manufacturing industry
04	Production processes
05	Extraction and distribution of fossil fuels and geothermal energy
06	Solvents and other product use
07	Road transport
08	Other mobile sources and machinery
09	Waste treatment and disposal
10	Agriculture
11	Other sources

New sources included

1) Traffic emission from small cities.

2) Agriculture and livestock emission coming from a top-down disaggregation EMEP emission database, specially in the case of NH_4^+ and NO_3^-.



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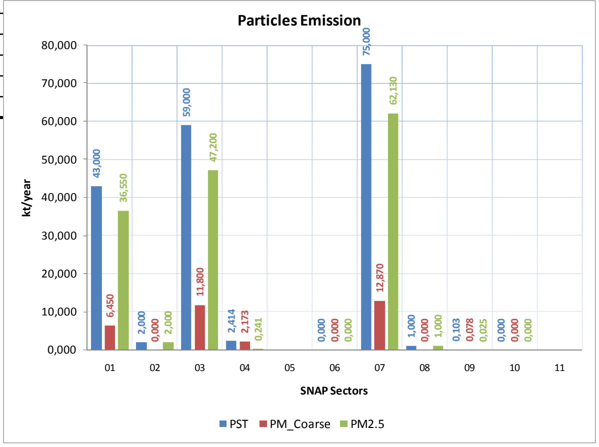
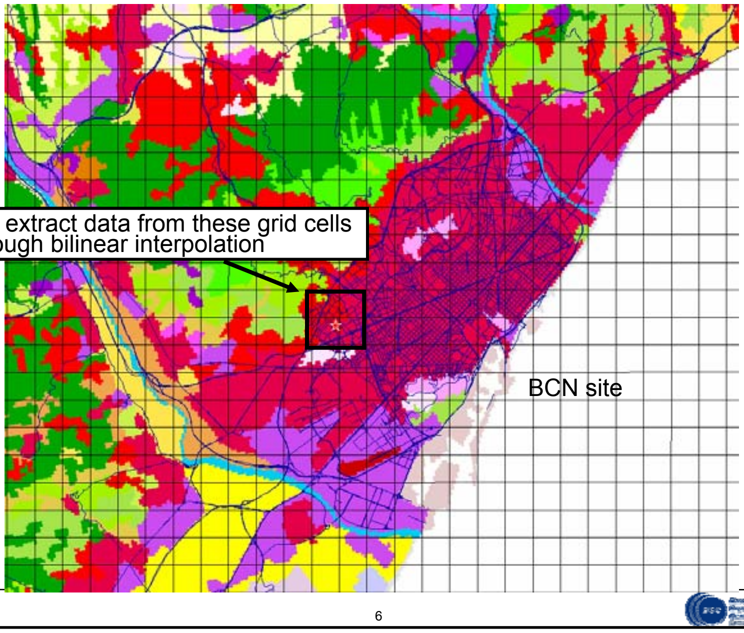
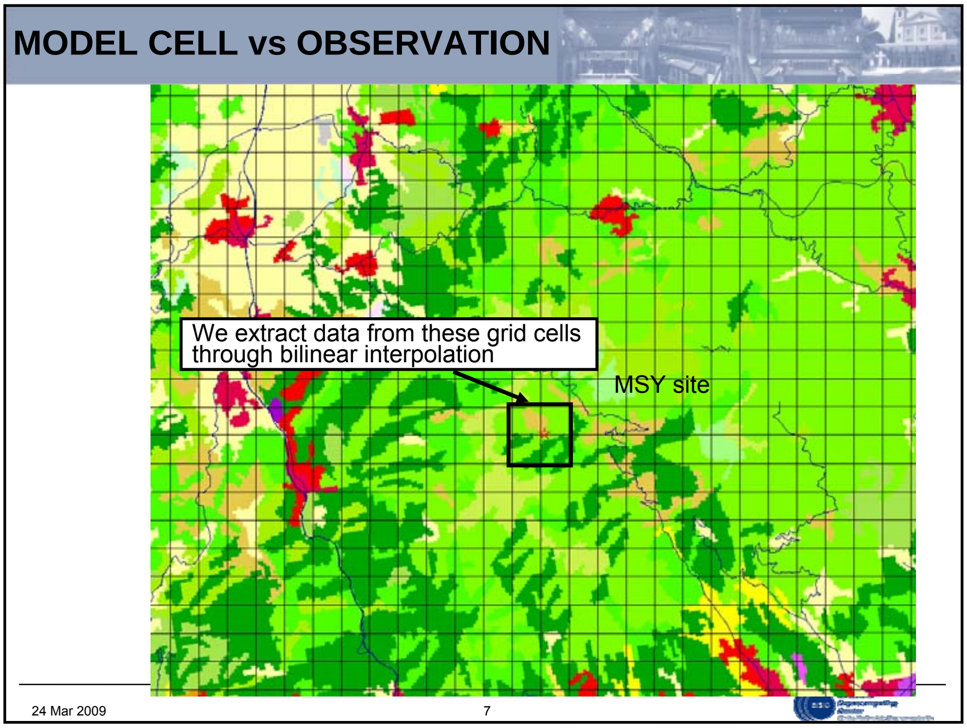


MODEL CELL vs OBSERVATION


We extract data from these grid cells through bilinear interpolation



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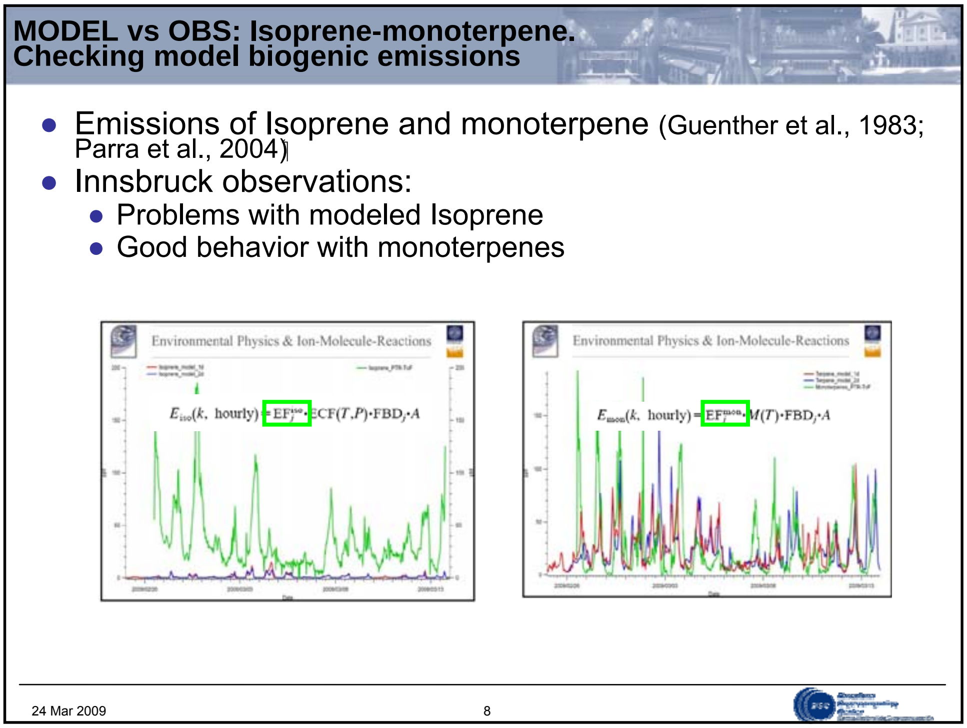

MODEL vs OBS: Isoprene-monoterpene. Checking model biogenic emissions

- Emissions of Isoprene and monoterpene (Guenther et al., 1983; Parra et al., 2004)
- Innsbruck observations:
  - Problems with modeled Isoprene
  - Good behavior with monoterpenes

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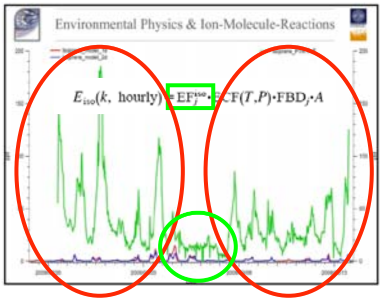

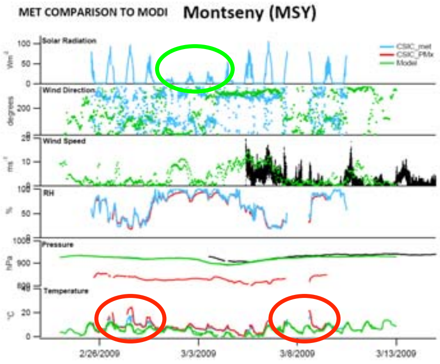

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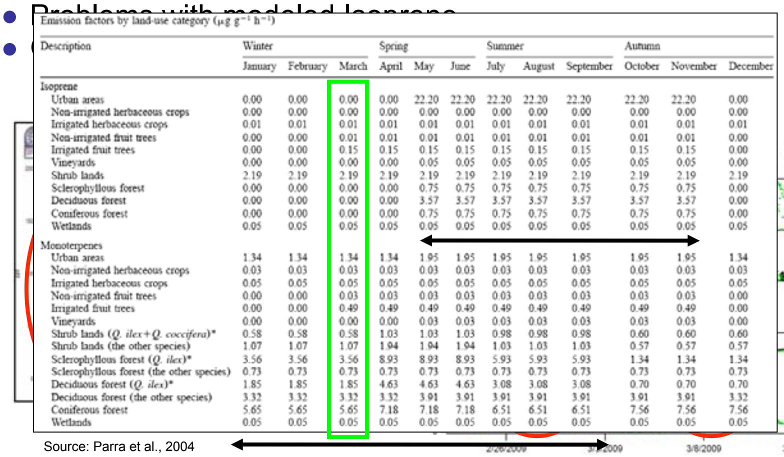
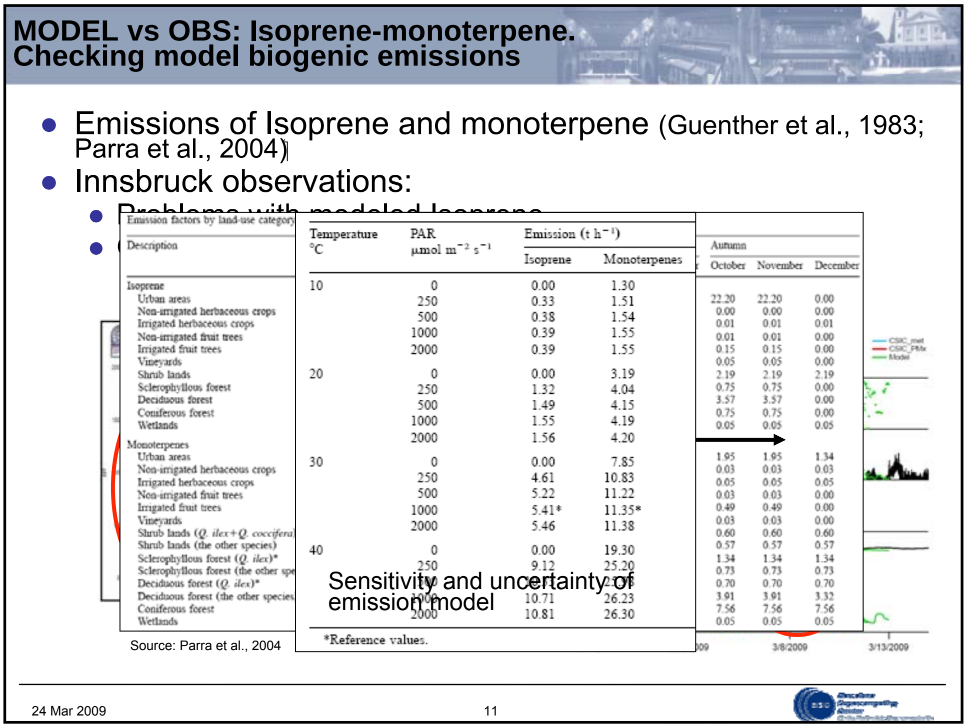


Emission factors by land-use category ($\mu g\ g^{-1}\ h^{-1}$)

Description	Winter			Spring			Summer			Autumn		
	January	February	March	April	May	June	July	August	September	October	November	December
Isoprene												
Urban areas	0.00	0.00	0.00	0.00	22.20	22.20	22.20	22.20	22.20	22.20	22.20	0.00
Non-irrigated herbaceous crops	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Irrigated herbaceous crops	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Non-irrigated fruit trees	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00
Irrigated fruit trees	0.00	0.00	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.00
Vineyards	0.00	0.00	0.00	0.00	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.00
Shrub lands	2.19	2.19	2.19	2.19	2.19	2.19	2.19	2.19	2.19	2.19	2.19	2.19
Sclerophyllous forest	0.00	0.00	0.00	0.00	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.00
Deciduous forest	0.00	0.00	0.00	0.00	3.57	3.57	3.57	3.57	3.57	3.57	3.57	0.00
Coniferous forest	0.00	0.00	0.00	0.00	0.75	0.75	0.75	0.75	0.75	0.75	0.75	0.00
Wetlands	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Monoterpenes												
Urban areas	1.34	1.34	1.34	1.34	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.34
Non-irrigated herbaceous crops	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
Irrigated herbaceous crops	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Non-irrigated fruit trees	0.00	0.00	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.00
Irrigated fruit trees	0.00	0.00	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.49	0.00
Vineyards	0.00	0.00	0.00	0.00	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.00
Shrub lands (*Q. ilex*+*Q. coccifera*)*	0.58	0.58	0.58	1.03	1.03	1.03	0.98	0.98	0.98	0.60	0.60	0.60
Shrub lands (the other species)	1.07	1.07	1.07	1.94	1.94	1.94	1.03	1.03	1.03	0.57	0.57	0.57
Sclerophyllous forest (*Q. ilex*)*	3.56	3.56	3.56	8.93	8.93	8.93	5.93	5.93	5.93	1.34	1.34	1.34
Sclerophyllous forest (the other species)	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73	0.73
Deciduous forest (*Q. ilex*)*	1.85	1.85	1.85	4.63	4.63	4.63	3.08	3.08	3.08	0.70	0.70	0.70
Deciduous forest (the other species)	3.32	3.32	3.32	3.32	3.91	3.91	3.91	3.91	3.91	3.91	3.91	3.32
Coniferous forest	5.65	5.65	5.65	7.18	7.18	7.18	6.51	6.51	6.51	7.56	7.56	7.56
Wetlands	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05

Source: Parra et al., 2004



MODEL vs OBS: Isoprene-monoterpene. Checking model biogenic emissions

- Emissions of Isoprene and monoterpene (Guenther et al., 1983; Parra et al., 2004)
- Innsbruck observations:
  - Problems with modeled Isoprene
  - (

Emission factors by land-use category

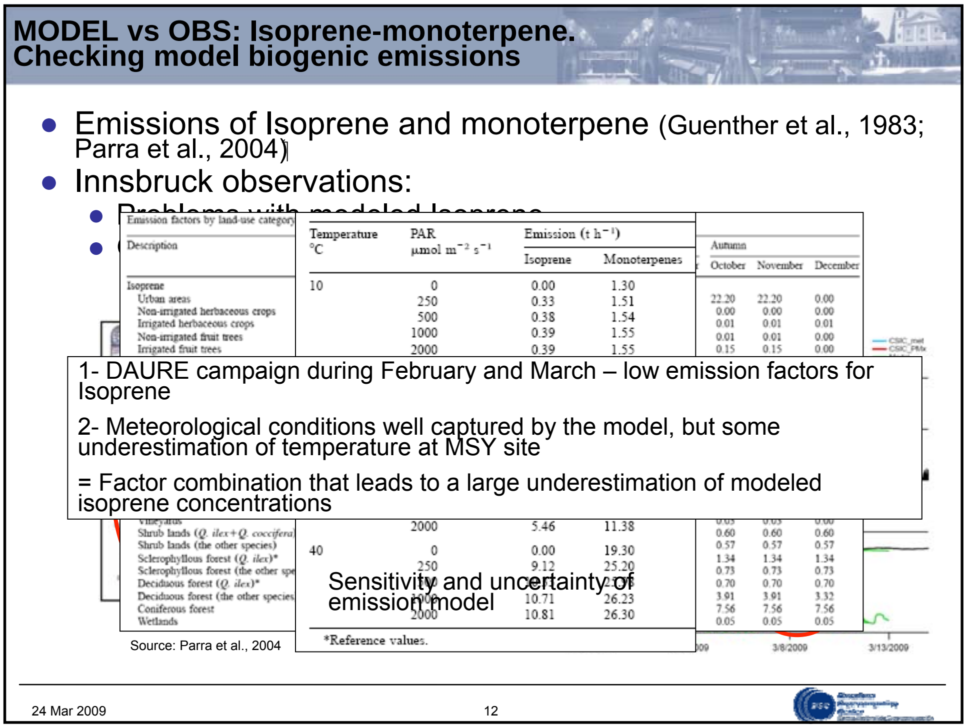
Description	October	November	December
Isoprene			
Urban areas	22.20	22.20	0.00
Non-irrigated herbaceous crops	0.00	0.00	0.00
Irrigated herbaceous crops	0.01	0.01	0.01
Non-irrigated fruit trees	0.01	0.01	0.00
Irrigated fruit trees	0.15	0.15	0.00
Vineyards	0.05	0.05	0.00
Shrub lands	2.19	2.19	2.19
Sclerophyllous forest	0.75	0.75	0.00
Deciduous forest	3.57	3.57	0.00
Coniferous forest	0.75	0.75	0.00
Wetlands	0.05	0.05	0.05
Monoterpenes			
Urban areas	1.95	1.95	1.34
Non-irrigated herbaceous crops	0.03	0.03	0.03
Irrigated herbaceous crops	0.05	0.05	0.05
Non-irrigated fruit trees	0.03	0.03	0.00
Irrigated fruit trees	0.49	0.49	0.00
Vineyards	0.03	0.03	0.00
Shrub lands (*Q. ilex*+*Q. coccifera*)	0.60	0.60	0.60
Shrub lands (the other species)	0.57	0.57	0.57
Sclerophyllous forest (*Q. ilex*)*	1.34	1.34	1.34
Sclerophyllous forest (the other spe	0.73	0.73	0.73
Deciduous forest (*Q. ilex*)*	0.70	0.70	0.70
Deciduous forest (the other species	3.91	3.91	3.32
Coniferous forest	7.56	7.56	7.56
Wetlands	0.05	0.05	0.05

Source: Parra et al., 2004

Temperature °C	PAR µmol m^{-2} s^{-1}	Emission (t h^{-1}) Isoprene	Emission (t h^{-1}) Monoterpenes
10	0	0.00	1.30
	250	0.33	1.51
	500	0.38	1.54
	1000	0.39	1.55
	2000	0.39	1.55
20	0	0.00	3.19
	250	1.32	4.04
	500	1.49	4.15
	1000	1.55	4.19
	2000	1.56	4.20
30	0	0.00	7.85
	250	4.61	10.83
	500	5.22	11.22
	1000	5.41*	11.35*
	2000	5.46	11.38
40	0	0.00	19.30
	250	9.12	25.20
	[illegible]	[illegible]	[illegible]
	1000	10.71	26.23
	2000	10.81	26.30

*Reference values.

Sensitivity and uncertainty of emission model



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- Emissions of Isoprene and monoterpene (Guenther et al., 1983; Parra et al., 2004)
- Innsbruck observations:
  - Problems with modeled Isoprene
  - (

1- DAURE campaign during February and March – low emission factors for Isoprene

2- Meteorological conditions well captured by the model, but some underestimation of temperature at MSY site

= Factor combination that leads to a large underestimation of modeled isoprene concentrations

Emission factors by land-use category

Description	October	November	December
Isoprene			
Urban areas	22.20	22.20	0.00
Non-irrigated herbaceous crops	0.00	0.00	0.00
Irrigated herbaceous crops	0.01	0.01	0.01
Non-irrigated fruit trees	0.01	0.01	0.00
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Vineyards			
Shrub lands (*Q. ilex*+*Q. coccifera*)	0.60	0.60	0.60
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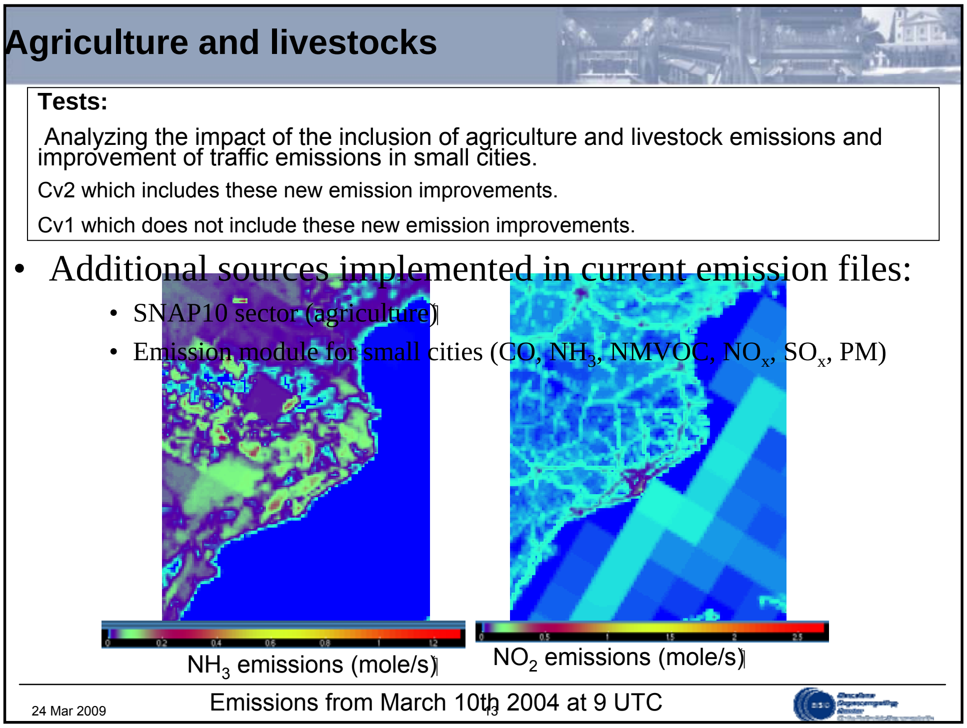


Agriculture and livestocks

Tests:

Analyzing the impact of the inclusion of agriculture and livestock emissions and improvement of traffic emissions in small cities.

Cv2 which includes these new emission improvements.

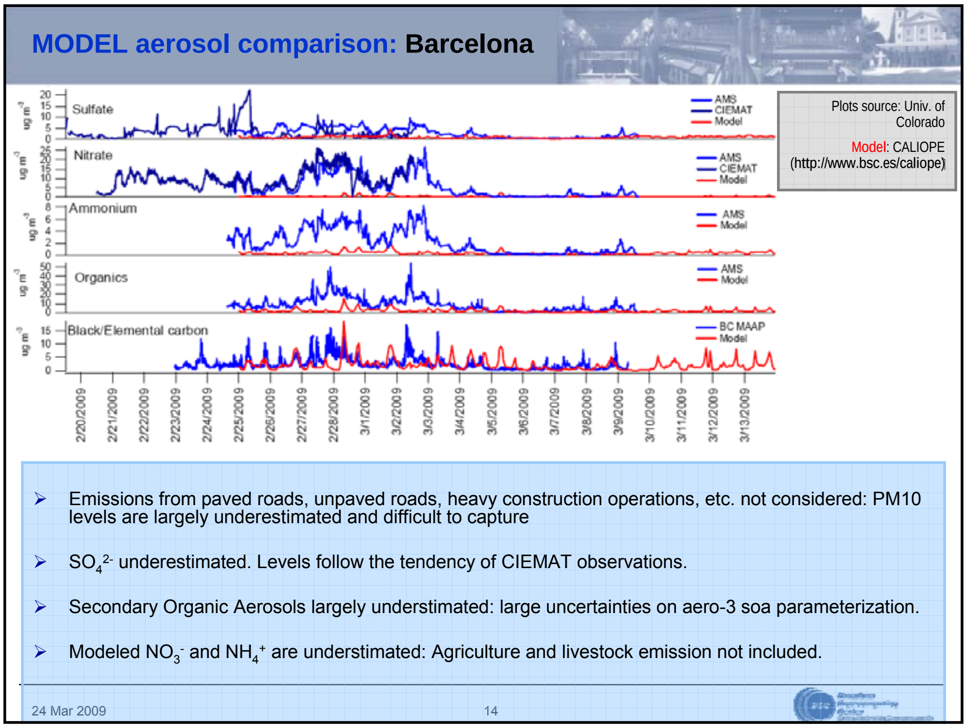
Cv1 which does not include these new emission improvements.

- Additional sources implemented in current emission files:
  - SNAP10 sector (agriculture)
  - Emission module for small cities (CO, NH_3, NMVOC, NO_x, SO_x, PM)

NH_3 emissions (mole/s)

NO_2 emissions (mole/s)

Emissions from March 10th 2004 at 9 UTC

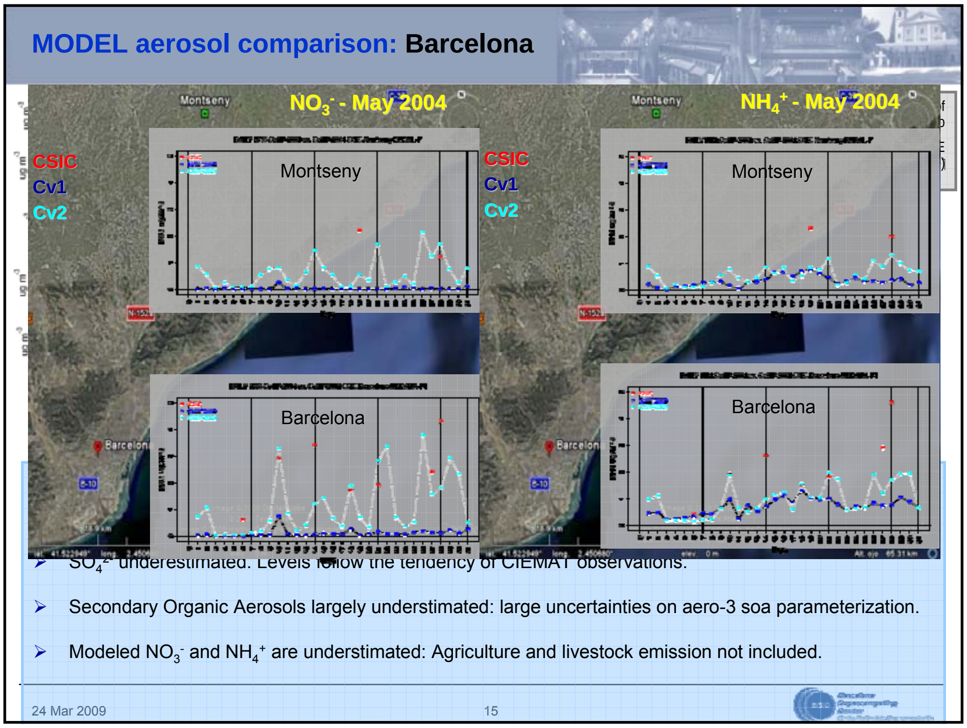


MODEL aerosol comparison: **Barcelona**

Plots source: Univ. of Colorado

Model: CALIOPE (http://www.bsc.es/caliope)

- Emissions from paved roads, unpaved roads, heavy construction operations, etc. not considered: PM10 levels are largely underestimated and difficult to capture
- SO_4^{2-} underestimated. Levels follow the tendency of CIEMAT observations.
- Secondary Organic Aerosols largely understimated: large uncertainties on aero-3 soa parameterization.
- Modeled NO_3^- and NH_4^+ are understimated: Agriculture and livestock emission not included.



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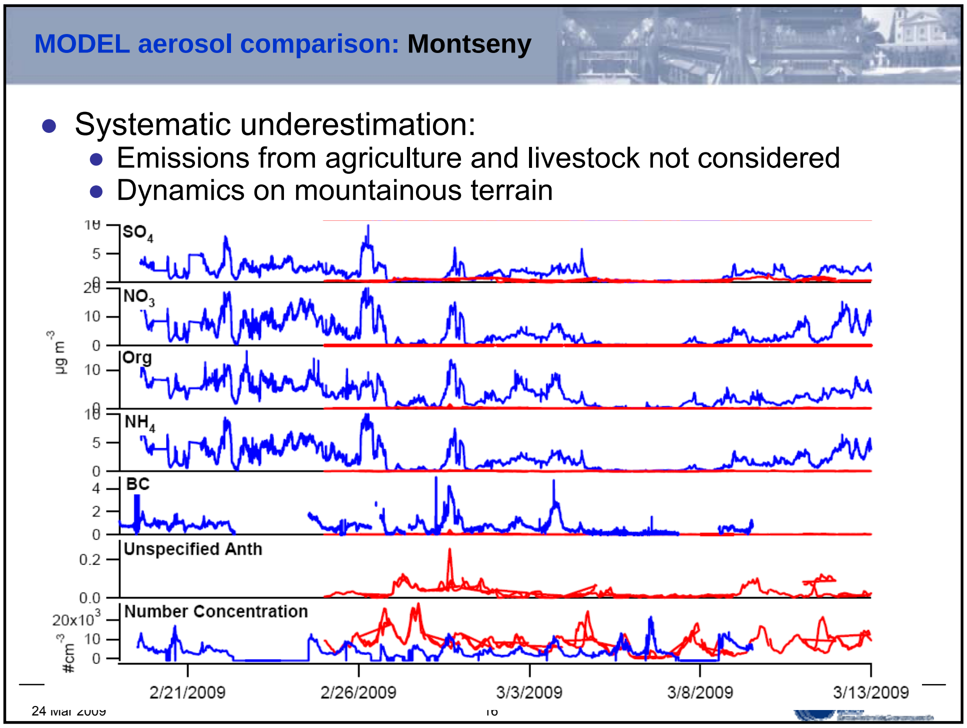

MODEL aerosol comparison: **Montseny**

- Systematic underestimation:
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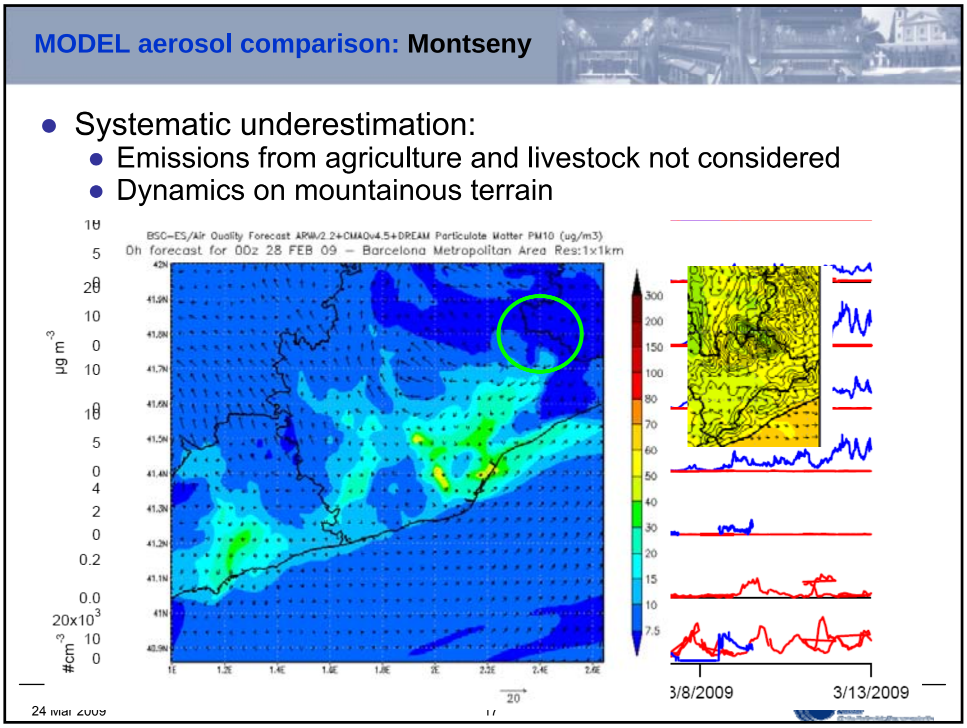
  - Dynamics on mountainous terrain



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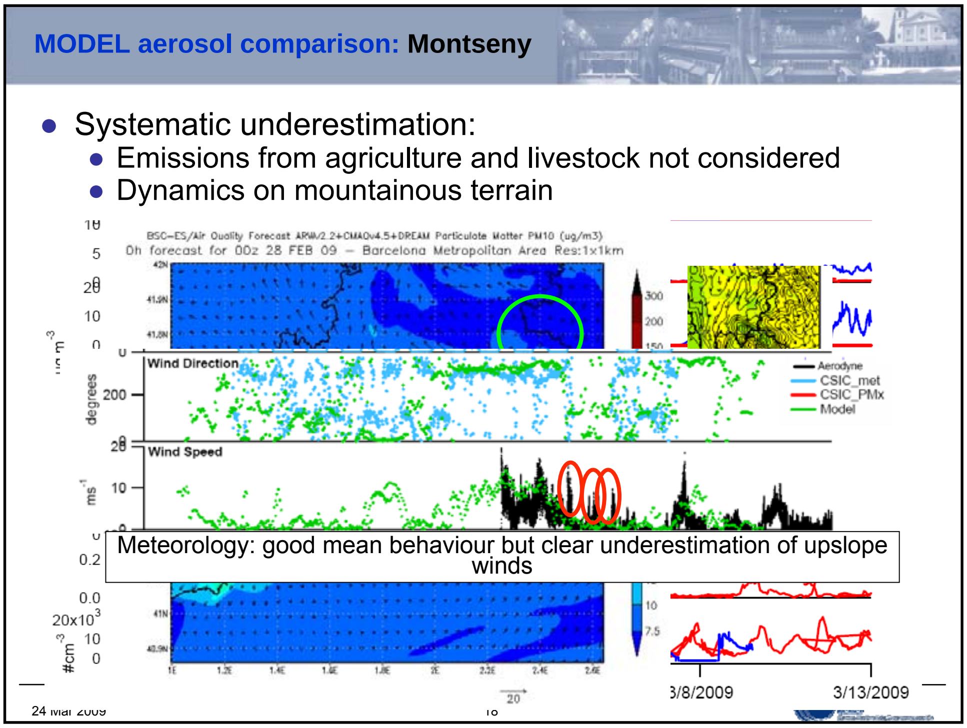

MODEL aerosol comparison: **Montseny**

- Systematic underestimation:
  - Emissions from agriculture and livestock not considered
  - Dynamics on mountainous terrain

Meteorology: good mean behaviour but clear underestimation of upslope winds

Comparison with other modeling studies

References	Summary of evaluation studies
Tonnesen, 2003	VISTAS and WRAP model comparison. SO_4^{2-} performance reasonably well. NO_3^- levels showed discrepancies, may need better NH_3 emissions.
Boyland and Baker, 2004	CAMx4, CMAQ-CB4, CMAQ-SARP99 comparison. SO_4^{2-} were more consistent among the three models; NO_3^- and organic matter have higher discrepancies.
Dennis, 2004	CMAQ evaluation. NO_3^- PM predictions are very sensitive to NH_x, and thus the NH_3 emissions need serious attention.
Morris et al.,2004a	CMAQ and CAMx did not perform well for NO_3^-. Better results are obtained for SO_4^{2-}.
Morris et al.,2004b	CAMx evaluation. SO_4^{2-} predictions were reasonable, but nitrate was significantly overpredicted.
Appel et al. 2008	CMAQ evaluation. Performance of NH_4^+ showed deficiencies in fall, which were related to NH_3 emission.
Yu et al. 2005	Model performance for NO_3^- is strongly dependent on model performance for NH_x, SO_4^{2-} and TNO_3

> *"The current performance of air quality models for PM is poor"…"There is a dire need for improving model inputs and model formulations in order to obtain acceptable model performance"…"3-D air quality models are the best tools available to address the PM source-receptors relationships because they take into account the non-linearities that affect the formation of secondary PM"*
>
> Seigneur, 2003.

Future tasks

- Improve emission sources:
  - Agriculture and livestock emissions
  - Sea salt aerosols
  - Mineral dust from European continent
  - Fugitive emissions: paved road emissions
  - Impact of water content
- Implement the new DREAM model configuration (size distribution 8 bins).
- Provide an updated model simulation for the DAURE campaign:
  - Hindcast simulation
  - New emission updates
  - CMAQv4.7 – CB05-aero4
- Run some tests proposed by José Luis concerning NH_3 model sensitivity

Papers proposal

- As leading authors:
  - Modeling evaluation of aerosol chemical speciation in the northeastern Spain: results from the DAURE campaign
- As contributors:
  - Those papers requiring further analysis and model sensitivity runs.

Thanks for your attention