9th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes

A FOUR MODEL INTERCOMPARISON CONCERNING CHEMICAL MECHANISMS AND NUMERICAL INTEGRATION METHODS

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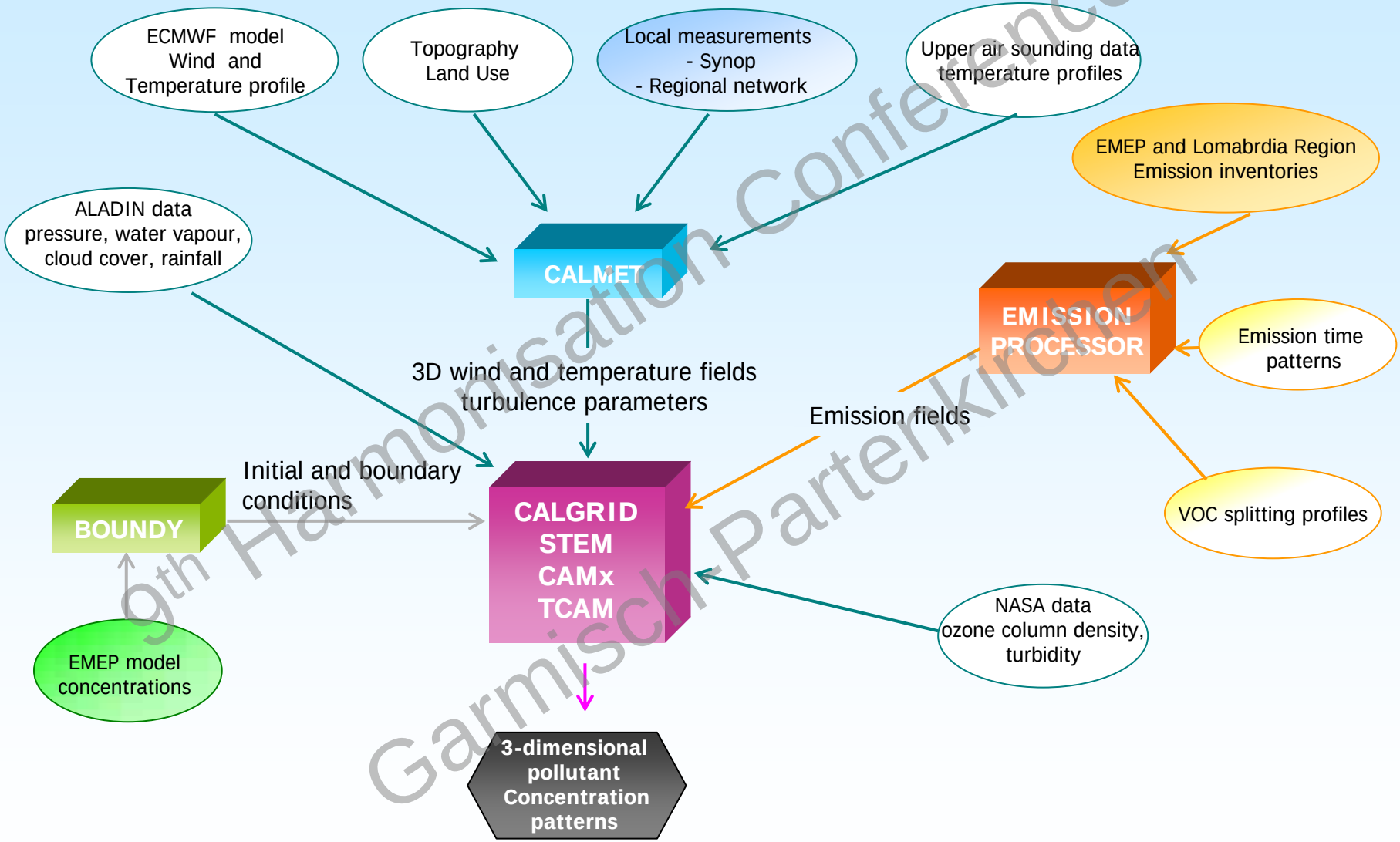
arpa SMR **EPA of Emilia Romagna Region**
CESI **CESI Research Centre**
D.E.A. University of Brescia
Council of Milan

Model Description (1/3)



Model Description (2/3)

Eulerian photochemical transport and dispersion models

CALGRID

- Modules for horizontal and vertical **advection/diffusion** (Chapeau Function)
- Resistance Based **Dry Deposition** Scheme
- Chemistry
  - Mechanism: **SAPRC90 and CBIV90**
  - Solver: **QSSA**

STEM-FCM

- Modules for horizontal and vertical **advection/diffusion** (Chapeau Function)
- Resistance Based **Dry Deposition** Scheme
- Photolysis rates adjusted as a function of cloud cover
- Wet Deposition
- Chemistry
  - Mechanism**: SAPRC90** (with explicit isoprene)
  - Solver**: IEH**

Model Description (3/3)

Eulerian photochemical transport and dispersion models

CAMx

- Modules for horizontal and vertical **advection/diffusion** (Bott Scheme)
- Resistance Based **Dry Deposition**
- Wet Deposition
- Photolysis rates adjusted as a function of cloud cover, total ozone column and turbidity
- Chemistry
  - Mechanism: **SAPRC99** and **CBIV99**
  - Solver: **CMC and IEH**

TCAM

- Modules for horizontal and vertical **advection/diffusion** (Chapeau Function)
- Resistance Based **Dry Deposition**
- Chemistry
  - Mechanism: **SAPRC90, SAPRC97, COCOH97** and **CBIV90**
  - Solver: **IEH**

Model Configuration

Model	Chemical Mechanism	Numerical Integrator
STEM	SAPRC 90	IEH
CALGRID	SAPRC 90	QSSA
CAMX	SAPRC99	CMC
CAMX	CBIV 99	CMC
TCAM	CBIV 90	IEH

Solvers&Chemistry (1/2)

- **QSSA (Quasi Steady State Approximation)**
  - Explicit Solver
- **IEH (Implicit-Explicit Hybrid Solver)**
  - Fast species: Implicit Method (LSODE)
  - Slow species: Explicit Method
  - Radicals: Steady State approx

Fast Species & Slow Species group fixed during the simulation

- **CMC (Chemical Mechanism Compiler)**
  - Fast species: Implicit Method (RK)
  - Slow species: Explicit Method
  - Radical: Steady State approx

NO, NO_2, O_3: always Fast
PAN: Fast if
conc>0.1*conc(NO_2)

Solvers&Chemistry (2/2)

Lumped Molecule

SAPRC90:
- 54 species
  - 40 state gasses
  - 14 radicals
- 128 reactions

SAPRC99:
- 74 Species
  - 56 state gasses
  - 18 radicals
- 211 Reactions

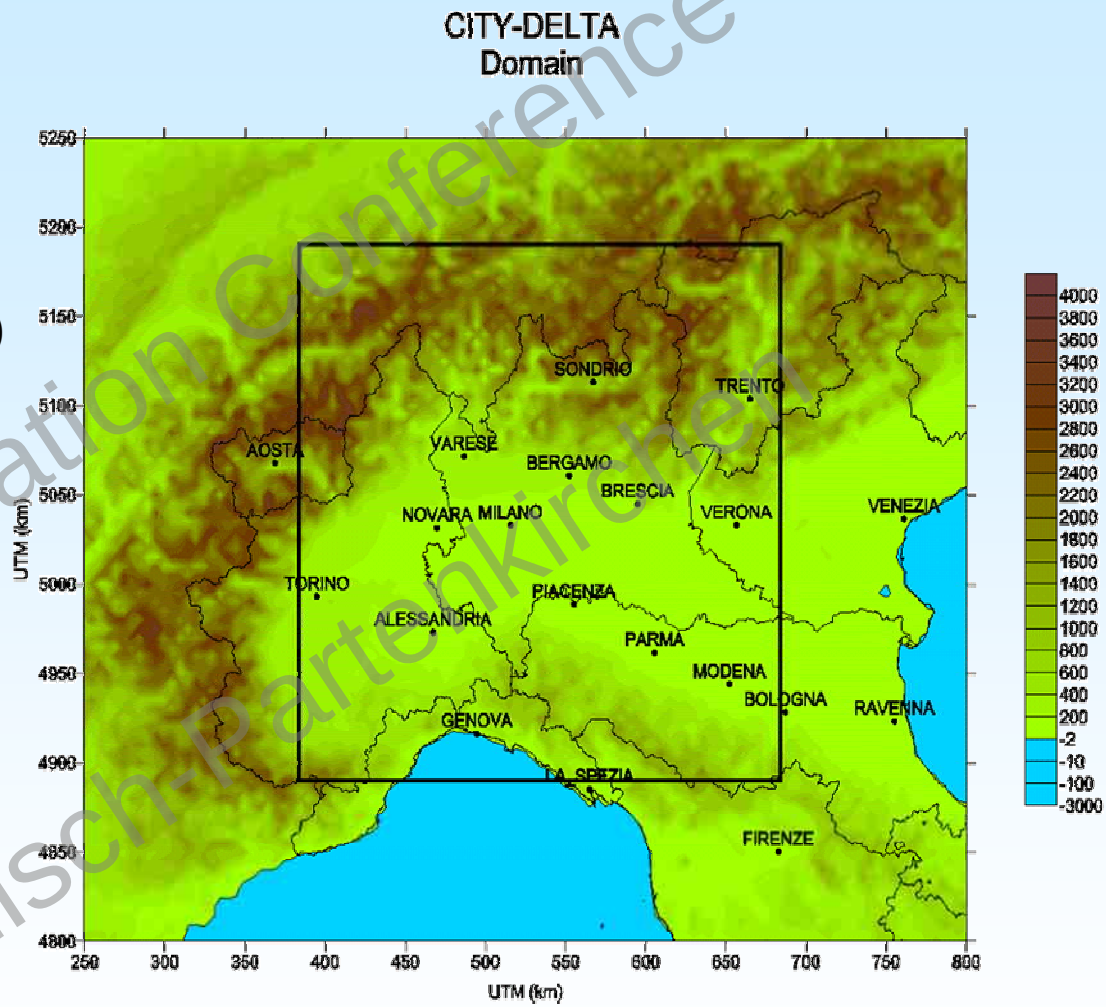
Lumped Structure

CBIV-90:
- 37 species
  - 25 state gasses
  - 12 radicals
- 85 reactions

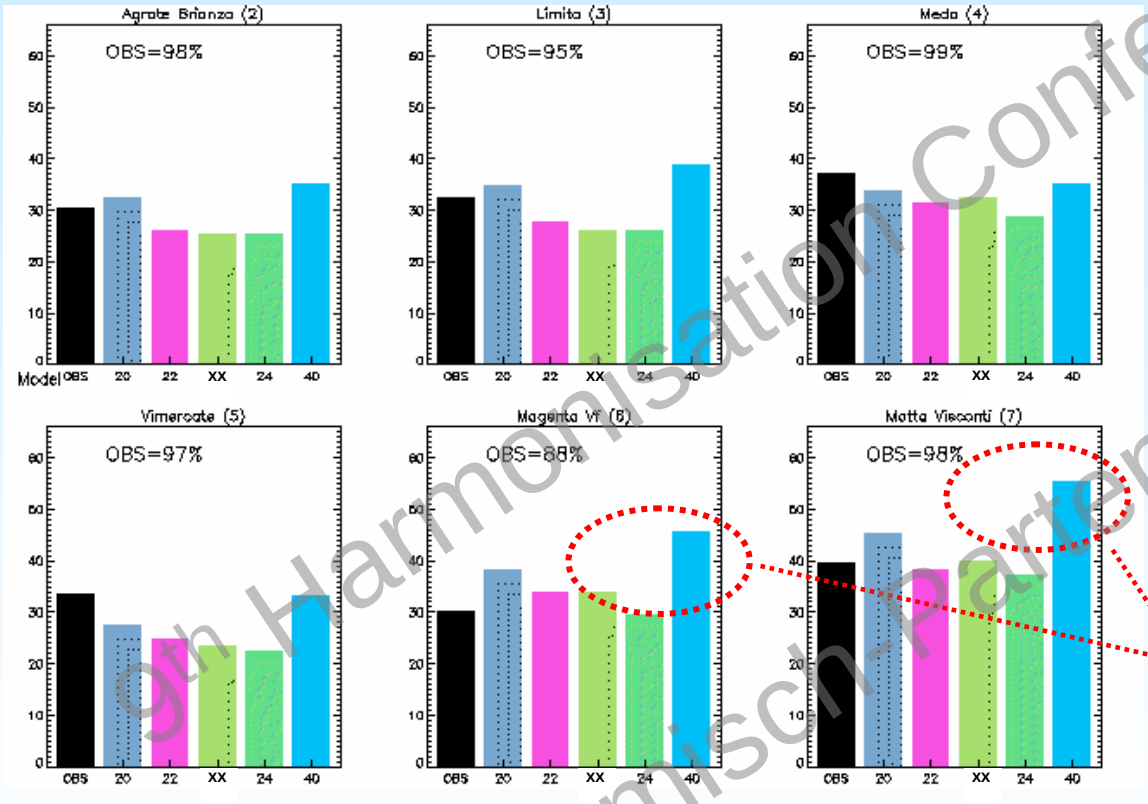
CBIV-99:
- 37 Species
  - 25 state gasses
  - 12 radicals
- 96 Reactions

Simulation Setup

- Area: 300x300 km^2 (Northern Italy)
- Horizontal resolution: 5x5 km^2
- Vertical Layers: 11
- Period: April-September 1999

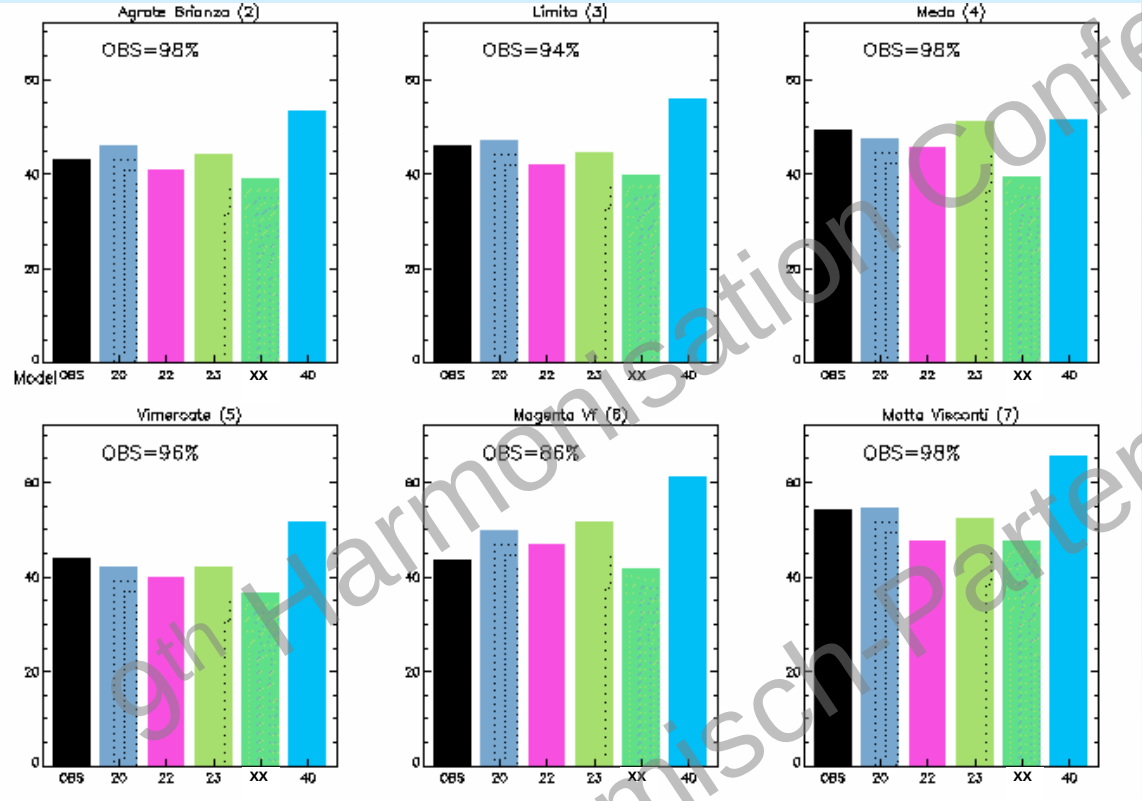


O3 Mean-T 0-24



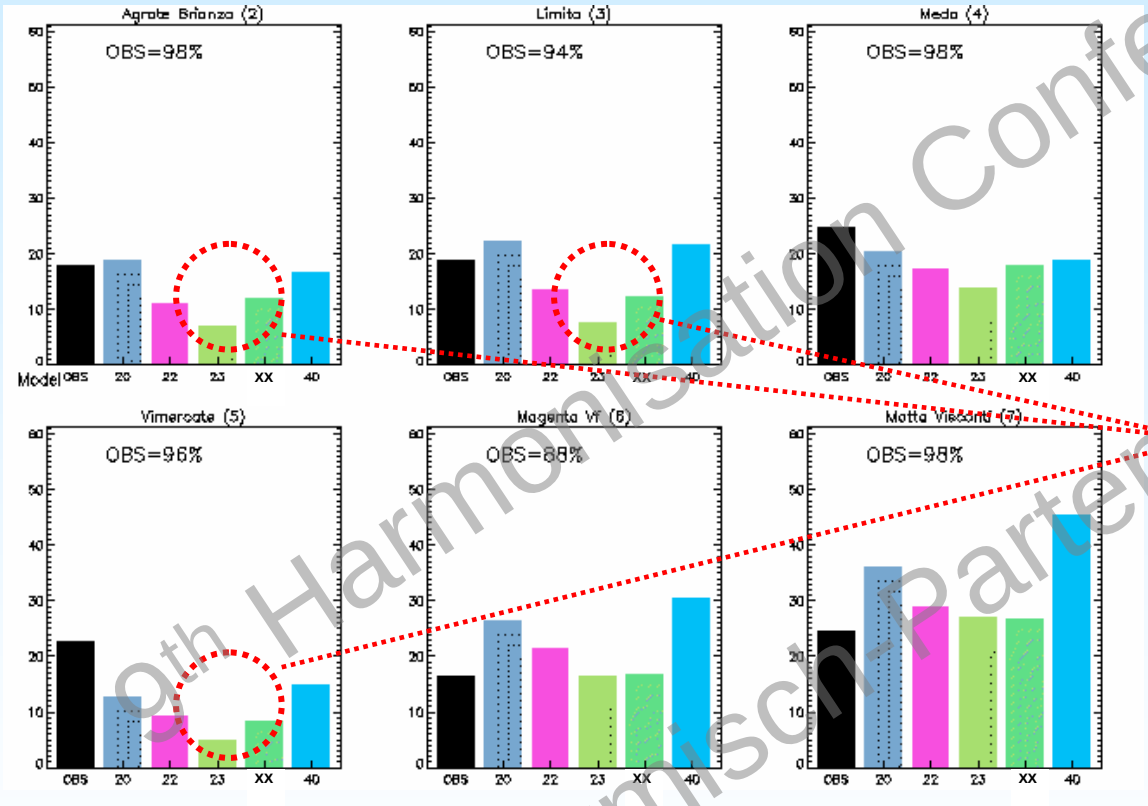
Model	Agreement
STEM (20)	
CALGRID (22)	
CAMX (23)	
CAMX (XX)	
TCAM (40)	

O3 Mean-T 8-20



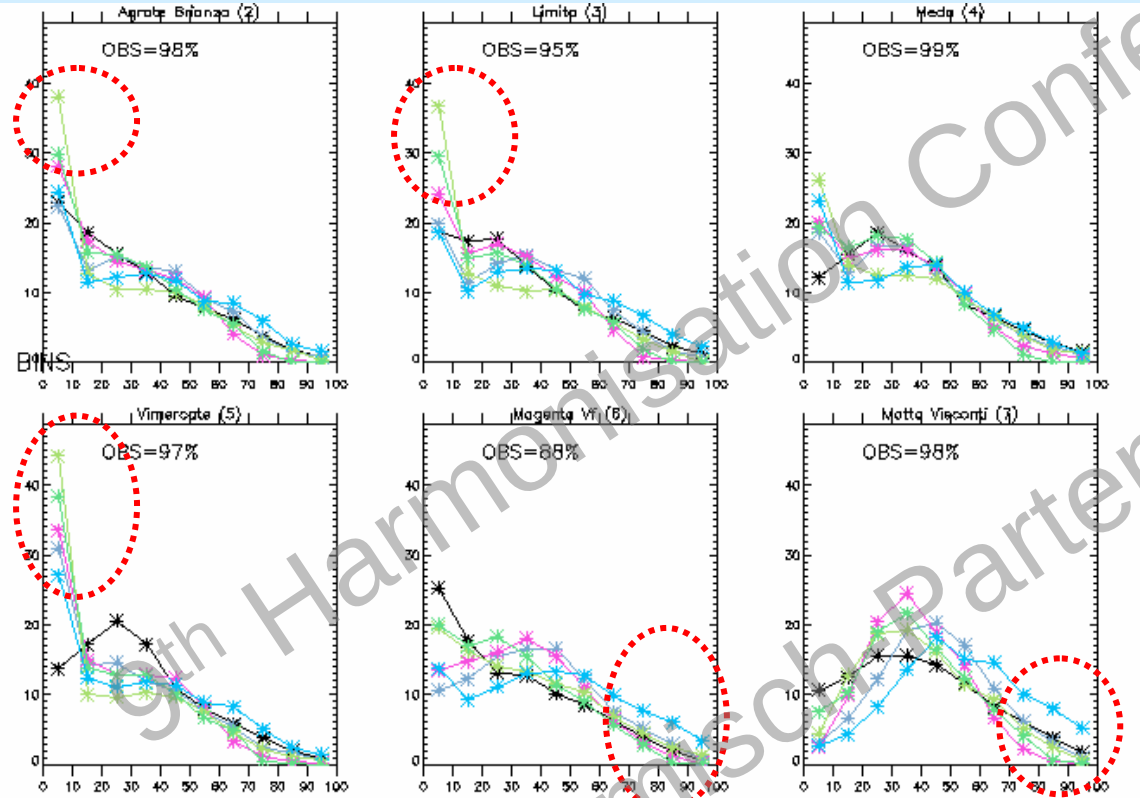
Model	Agreement
STEM (20)	
CALGRID (22)	
CAMX (23)	
CAMX (XX)	
TCAM (40)	

O3 Mean-T 20-8



Model	Agreement
STEM (20)	⬢
CALGRID (22)	⬢
CAMX (23)	⬢
CAMX (XX)	⬢
TCAM (40)	⬢

O3 Frequency 0-24



Model	Agreement
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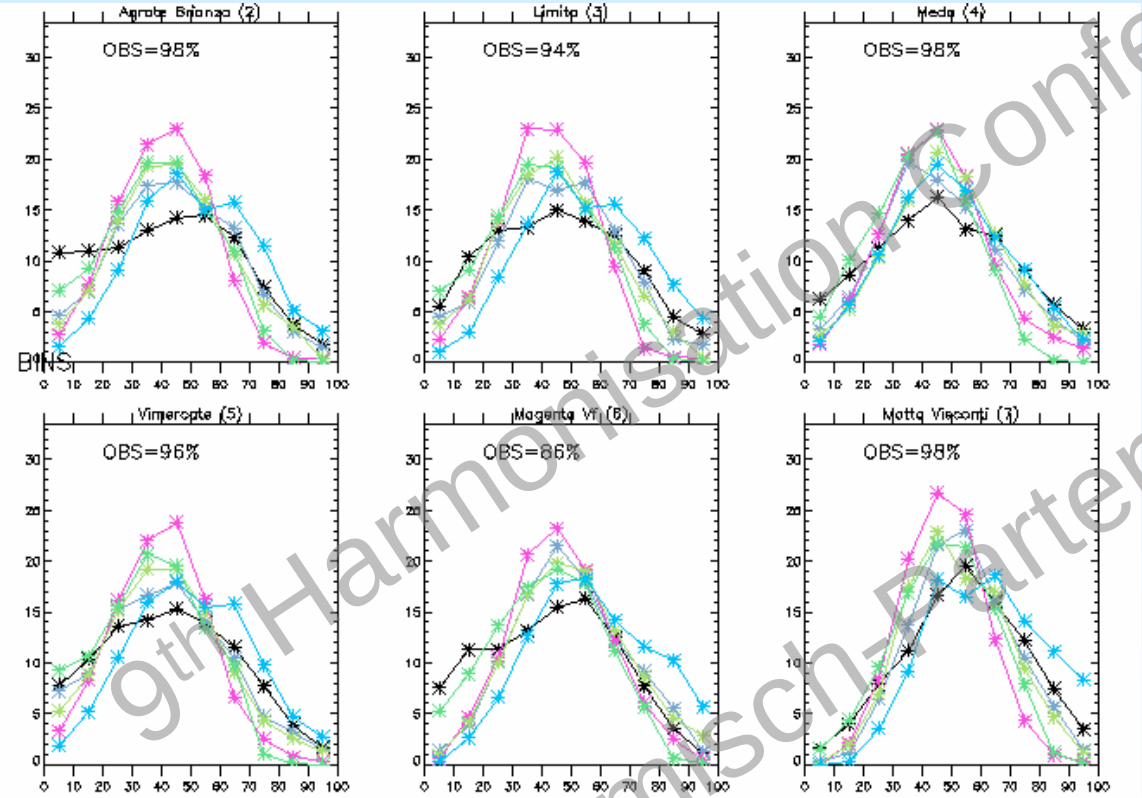
CALGRID (22)	
CAMX (23)	
CAMX (XX)	
TCAM (40)	

O3 Frequency 8-20



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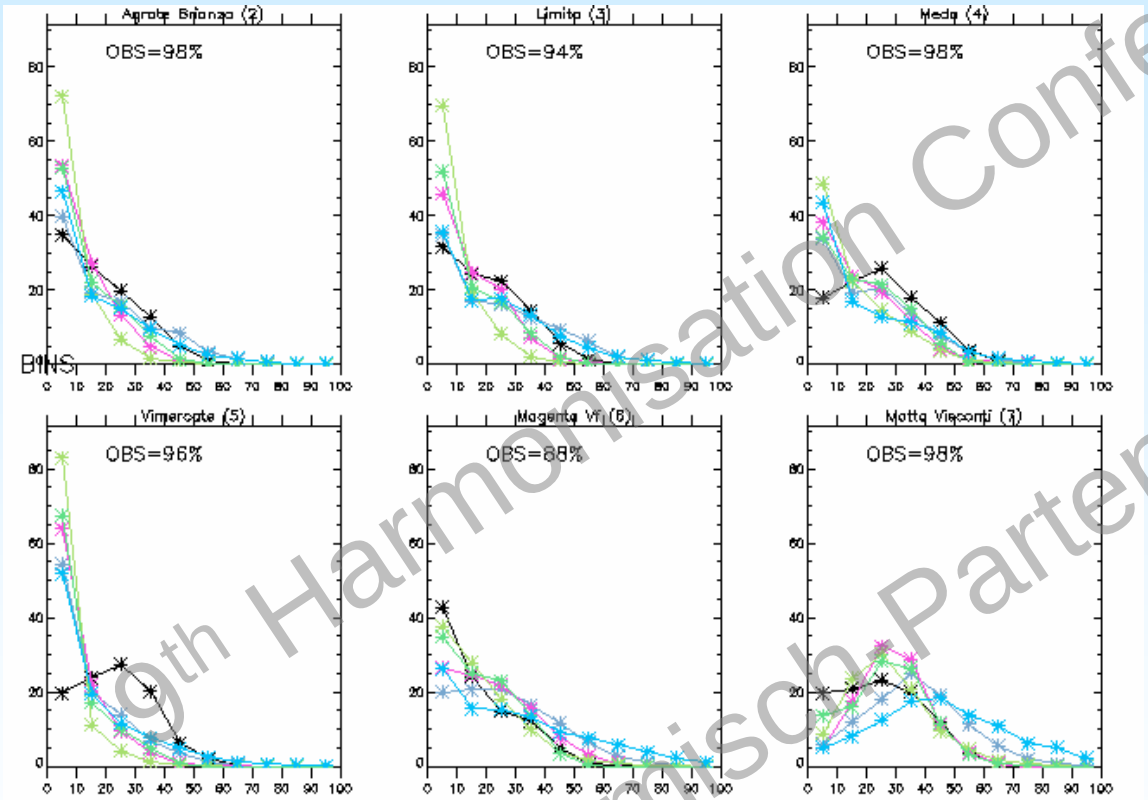
STEM (20)	
CALGRID (22)	
CAMX (23)	
CAMX (XX)	
TCAM (40)	

O3 Frequency 20-8



Model	Agreement
STEM (20)	
CALGRID (22)	
CAMX (23)	
CAMX (XX)	
TCAM (40)	

Validation Performance

Model	Chemical Mechanism	Numerical Integrator	Mean-T 0-24	Mean-T 8-20	Mean-T 20-8	Freq. 0-24	Freq. 8-20	Freq. 20-8
CAMX (XX)	CBIV99	CMC						
TCAM (40)	CBIV90	IEH						

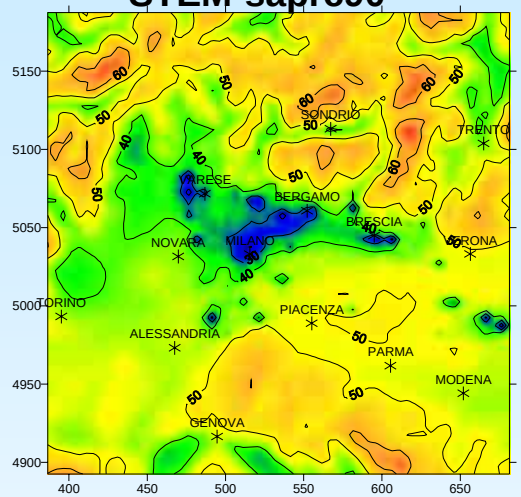
Model implementing CMC integrator:
- Day-time: concentrations calculated using **SAPRC99** are higher than **CBIV99**
- Night-time: concentrations are very similar

Models implementing IEH integrator:
- **TCAM** concentrations are higher than **STEM** ones
- **TCAM** overestimates concentrations higher than 70 ppb

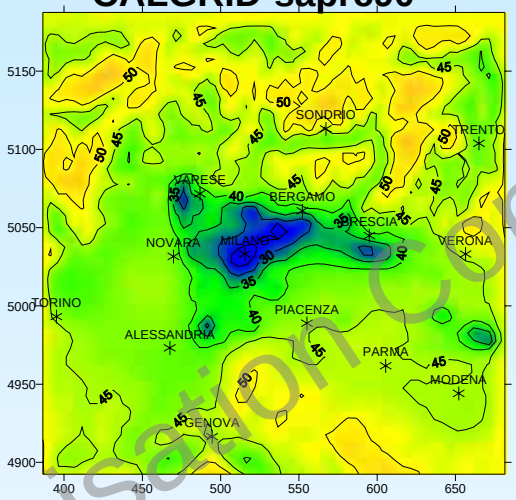
Models using SAPRC mechanisms:
- Mean Concentrations are **very similar**
- **IEH** ensures better performance than **QSSA**
- **IEH/CMC** have same performance during the day
- **IEH** is better than **CMC** during the night

O3 MeanT Fields

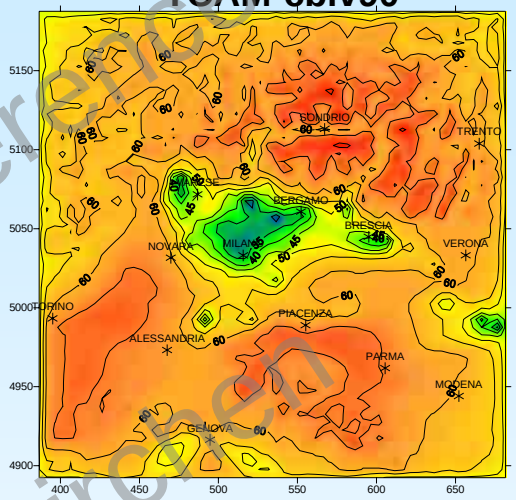
STEM-saprc90

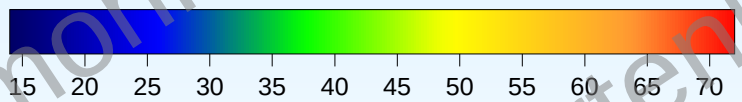


CALGRID-saprc90

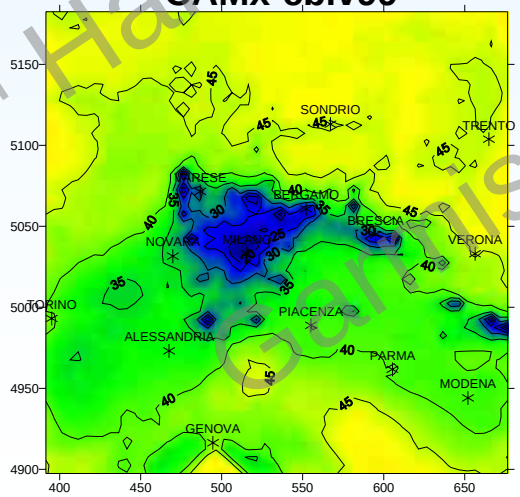


TCAM-cbiv90

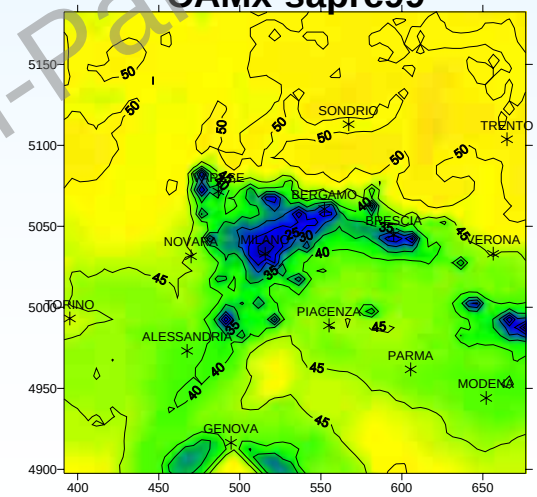




CAMx-cbiv99



CAMx-saprc99



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Conclusion

- All the configurations tested shows a good agreements with measures
- Solvers:
  - IEH generally shows better performances than CMC and QSSA
  - CMC works very well during the day (performances comparable to that IEH), but it underestimates ozone concentrations during the night
  - QSSA is not able to correctly reproduce higher concentration

- Mechanisms
  - Similar performance during the night
  - Similar mechanism => Similar spatial distribution ?

Thanks to…

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