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Comparative Analysis of Air Quality Models CIT, WRF-Chem and SPM-BRAMS for the Second Ozone Campaign in Metropolitan Area of São Paulo

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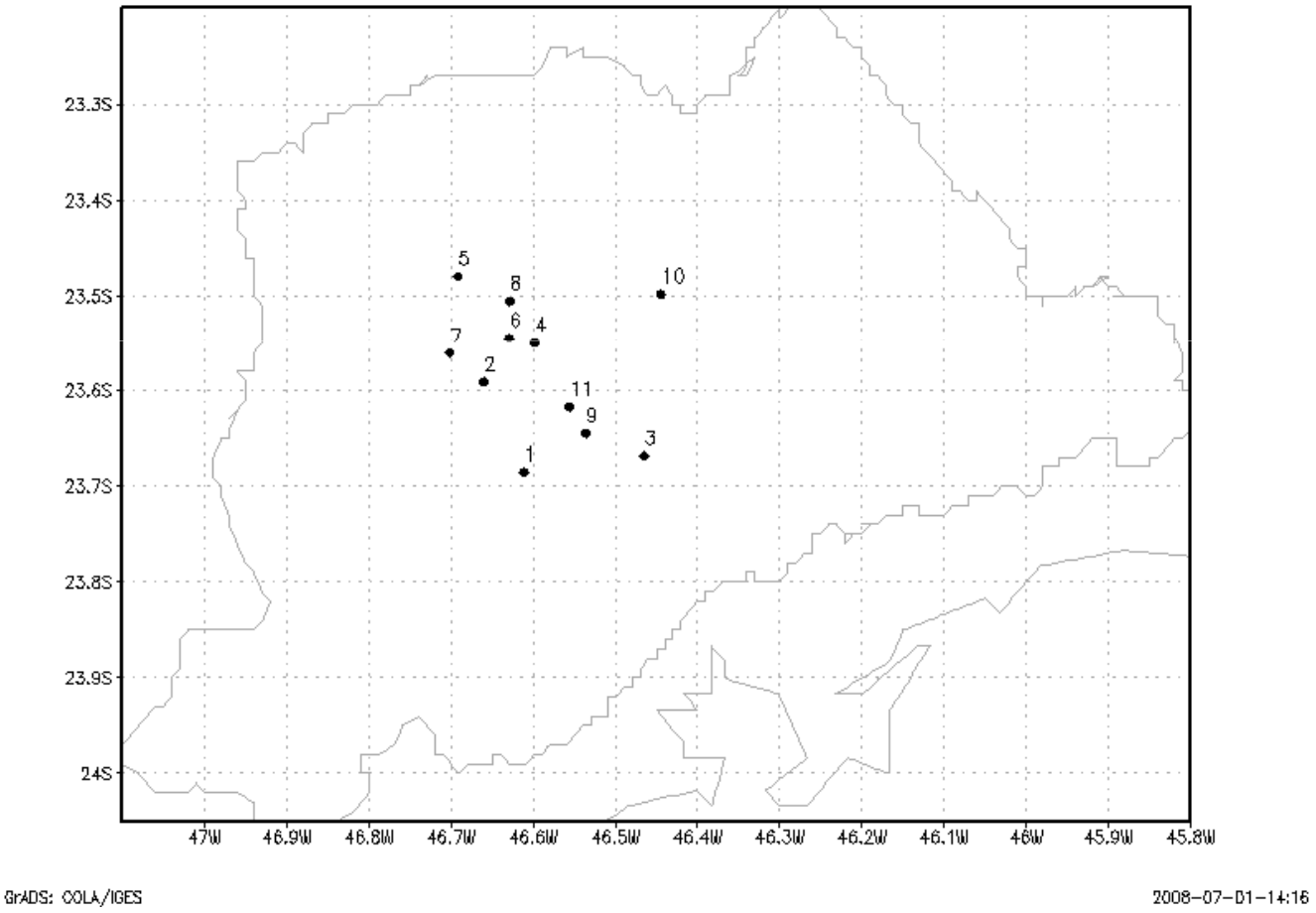
Introduction – MASP

- Urban Area: 8000 km^2;
- Population: 19 million people;
- Over 2000 Industries;
- More than 7 million vehicles:
  - 20% of the national fleet;
  - Large variety of fuels: gasohol (with 22% of ethanol and 78% of gasoline), hydrated ethanol, compressed natural gas (CNG), and diesel (Sánchez-Ccoyllo et al, 2006);
  - Responsible for: 97% of CO and HC emissions;
    96% of NO_X;
    40% of PM;
    42% of SO_X (CETESB, 2008).

Introduction – The Ozone Problems in the MASP

Ozone Monitoring Network in the MASP



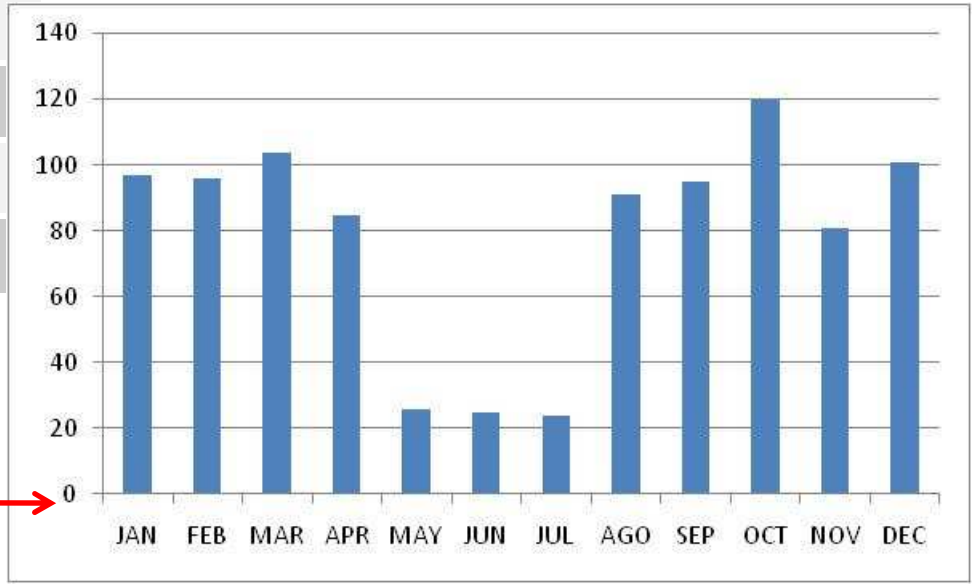
Introduction – The Ozone Problems in the MASP

Year	Nº of days of NAAQS exceedances
1999	80
2000	67
2001	78
2002	82
2003	77
2004	63
2005	51
2006	46
2007	72

CETESB, 2008.

NAAQS exceedances occurs during all year but specially during spring and summer time.

Monthly mean distribution of NAAQS exceedances (1996 – 2007)



Introduction – The Ozone Problems in the MASP

Hence, the use of photochemical air quality models can be an important tool specially to:

• Evaluate the air quality in the entire metropolitan area and in the surrounding regions which are not cover by the existing air quality monitoring network.

• Understand the ozone photochemistry in the area in order to help to establish goals and ways to address the problem.

Introduction – The Ozone Problems in the MASP

Photochemical air quality models started to be used in the MASP in the late 90's. Since then, several studies were developed in order to evaluate the performance of those models and to understand the photochemical process in the area.

The models mostly used so far were the CIT and the SPM-BRAMS. More recently the WRF-Chem model started to be used as well.

Objective

To evaluate the performance of different air quality models (off-line and in-line) to simulate ozone concentrations in the MASP. CO and NO_X concentrations results also were evaluated through comparison with monitoring data.

Air Quality Models Used

	CIT	WRF-Chem	SPM-BRAMS
Classification	Off-line	In-line	
Chemistry	**SAPRC99 223 reactions**	**RADM2 157 reactions**	**Based on SAPRC99 – Only 15 reactions**

SPM-BRAMS 15 Reactions

$NO + ½\ O_2 \rightarrow NO_2$

$NO_2 + \lambda v \rightarrow NO + O(^3P)$

$O(^3P) + O_2 + M \rightarrow O_3 + M$

$O_3 + NO \rightarrow NO_2 + O_2$

$O_3 + NO_2 \rightarrow O_2 + NO_3$

$O_3 + \lambda v \rightarrow O(^1D) + O_2$

$O(^1D) + H_2O \rightarrow 2\ OH\cdot$

$OH\cdot + CO \rightarrow HO_2\cdot + CO_2$

$HO_2\cdot + NO \rightarrow OH\cdot + NO_2$

$HO_2\cdot + O_3 \rightarrow OH\cdot + 2O_2$

Inorganic Reactions

$RH + OH\cdot \rightarrow H_2O + RO_2\cdot$

$RO_2\cdot + NO \rightarrow NO_2 + RCHO + HO_2\cdot$

$RCHO + OH\cdot \rightarrow RCO\text{-}O_2 + H_2O$

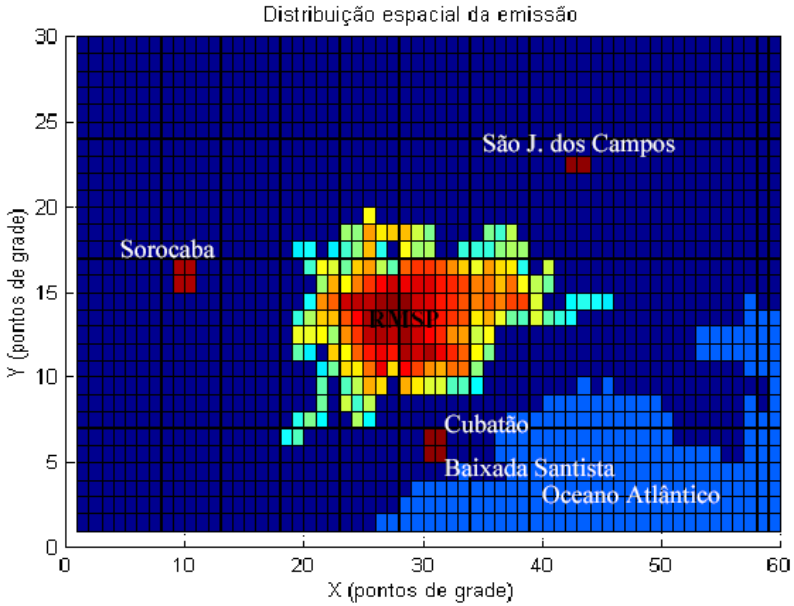
$HO_2\cdot + HO_2\cdot \rightarrow H_2O_2 + O_2$

$HO_2\cdot + RO_2\cdot \rightarrow ROOH$

Organic Reactions

VOC Lumping

Emission

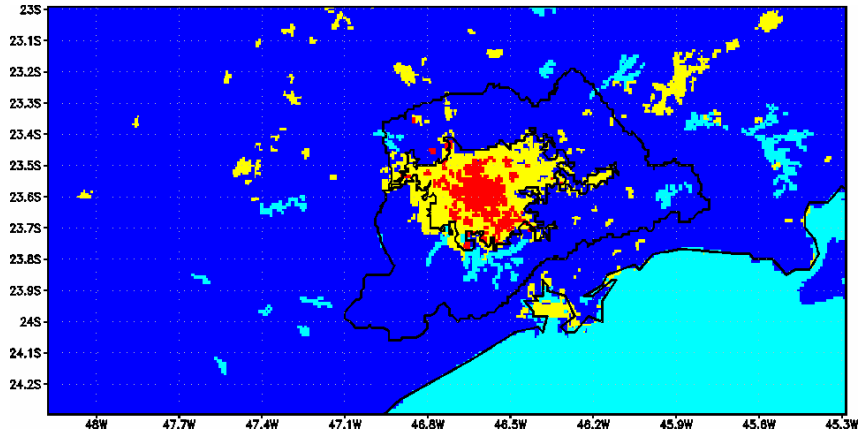


WRF-Chem and CIT

- Emission Rates for several compounds (estimated by tunnel measurements).
- Spatially distributed (5x5km).
- Hourly distributed.

SPM-BRAMS

- Emission Rate for only 6 compounds.
- Two types of Urban Areas responsible for 30% and 70% of emissions.
- Hourly distributed;
- Dependent of the day of the week.



Simulation details:

- From october 30 to november 01of 2006;

- SPM-BRAMS and WRF-Chem were started 24 hours early;

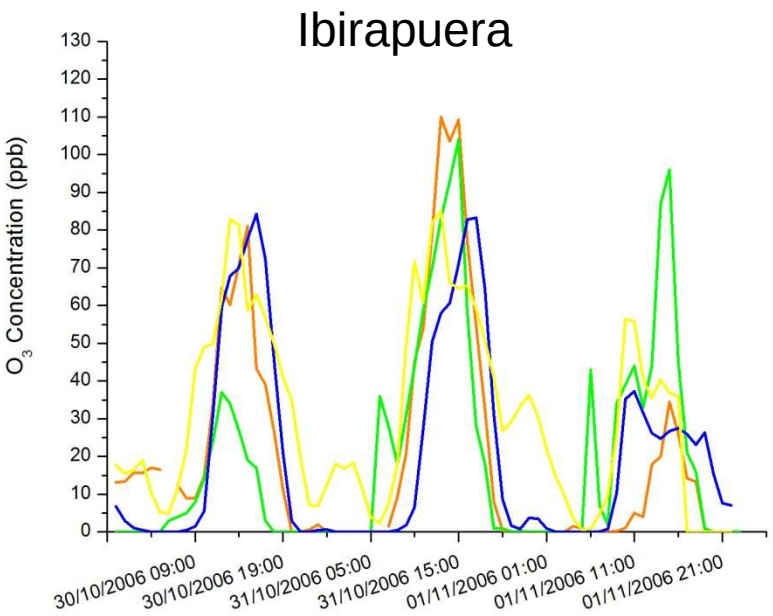
Grid:

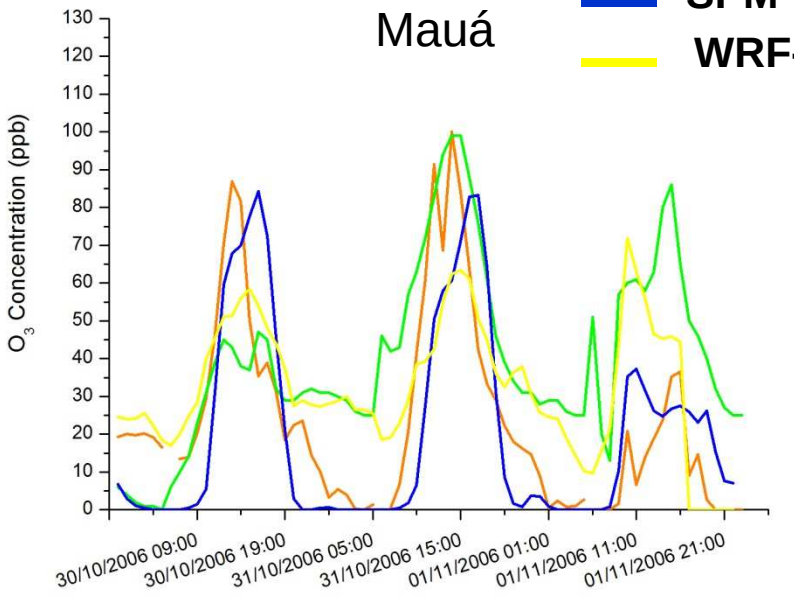
- Two nested grids (SPM-BRAMS) – 20 and 5 km
- One grid (CIT and WRF-Chem) – 5 km.

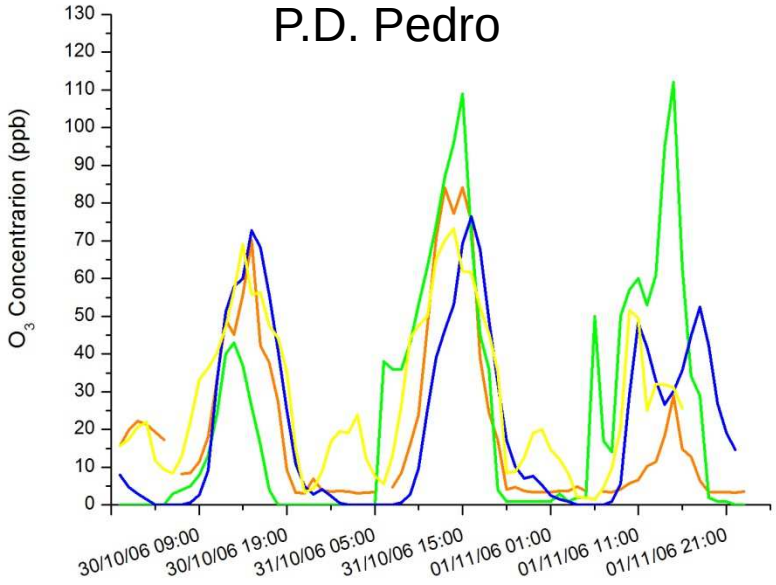
Second Ozone Monitoring Campaign - Between Oct 30 and Nov 1 .

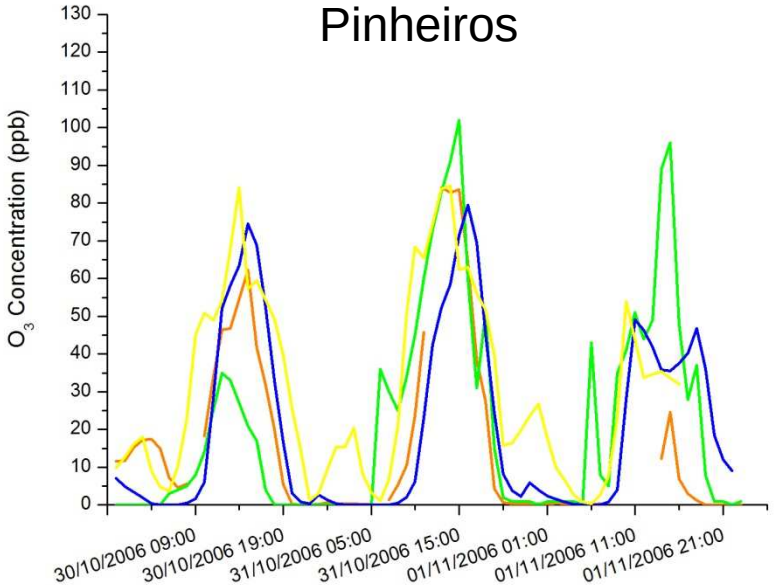
Results – O_3 Concentrations

CETESB
CIT
SPM-BRAMS
WRF-Chem





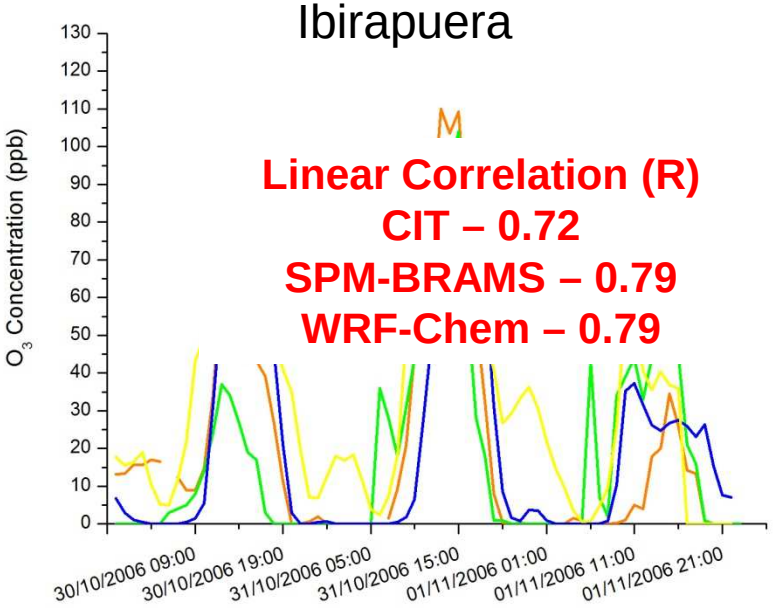




Results – O_3 Concentrations

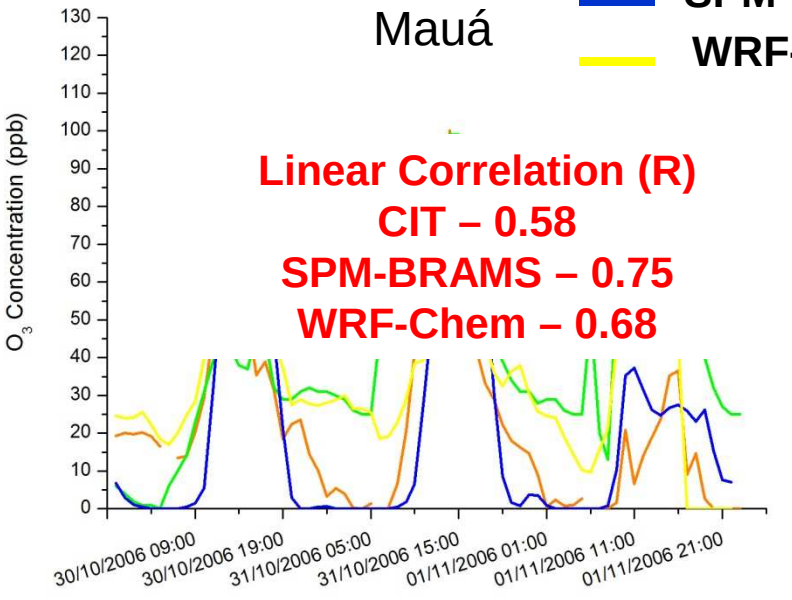
CETESB
CIT
SPM-BRAMS
WRF-Chem

Ibirapuera



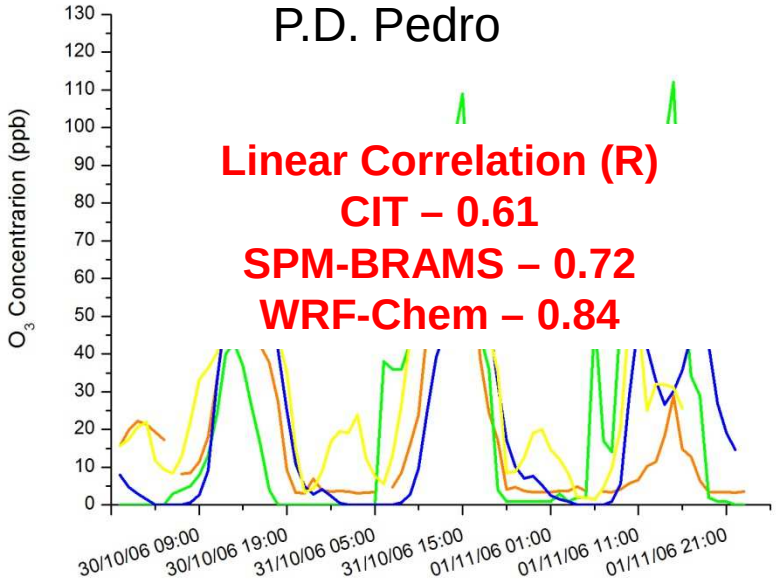
Linear Correlation (R)
CIT – 0.72
SPM-BRAMS – 0.79
WRF-Chem – 0.79

Mauá



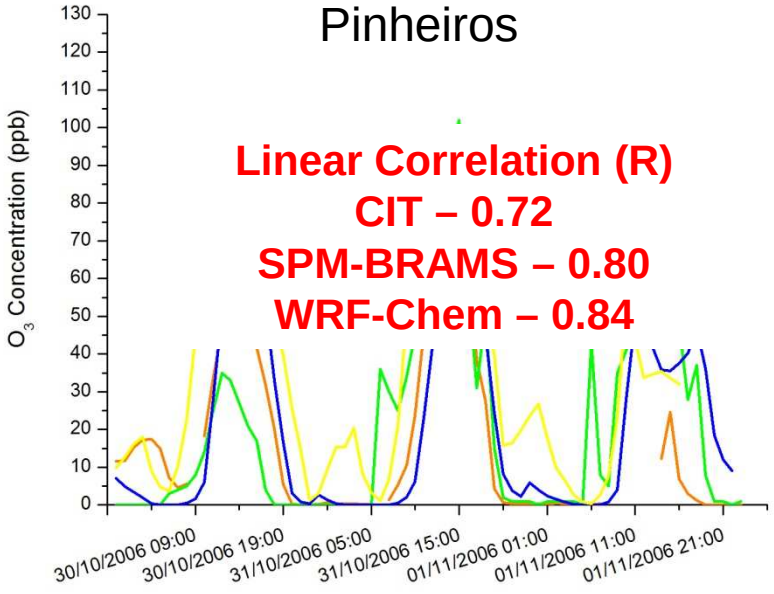
Linear Correlation (R)
CIT – 0.58
SPM-BRAMS – 0.75
WRF-Chem – 0.68

P.D. Pedro



Linear Correlation (R)
CIT – 0.61
SPM-BRAMS – 0.72
WRF-Chem – 0.84

Pinheiros

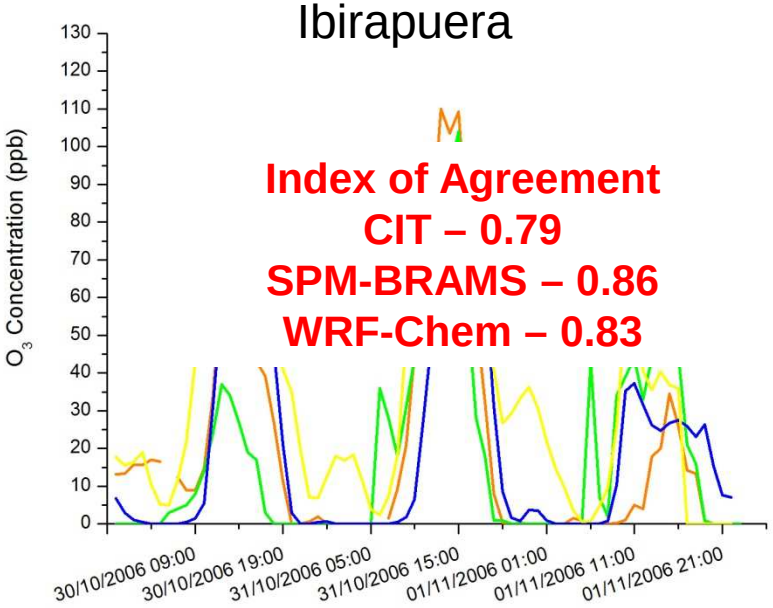


Linear Correlation (R)
CIT – 0.72
SPM-BRAMS – 0.80
WRF-Chem – 0.84

Results – O_3 Concentrations

CETESB
CIT
SPM-BRAMS
WRF-Chem

Ibirapuera



Index of Agreement
CIT – 0.79
SPM-BRAMS – 0.86
WRF-Chem – 0.83

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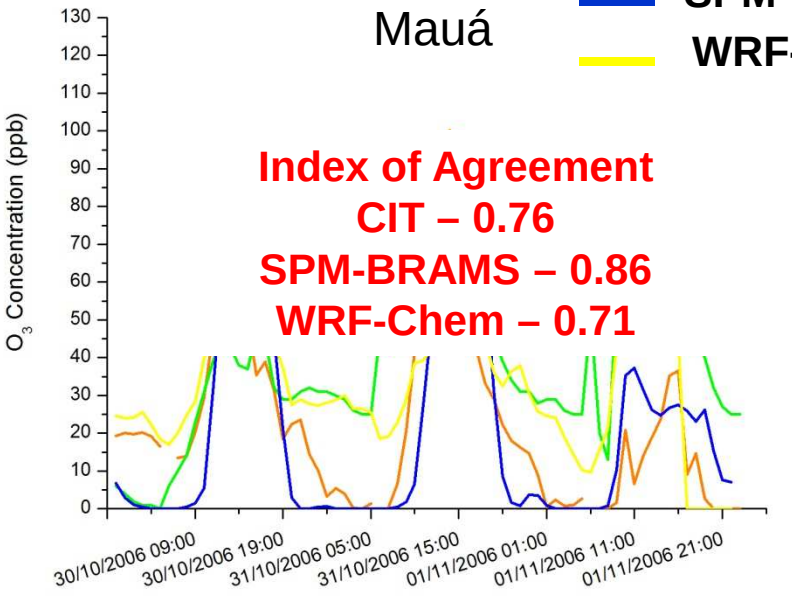

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CIT – 0.76
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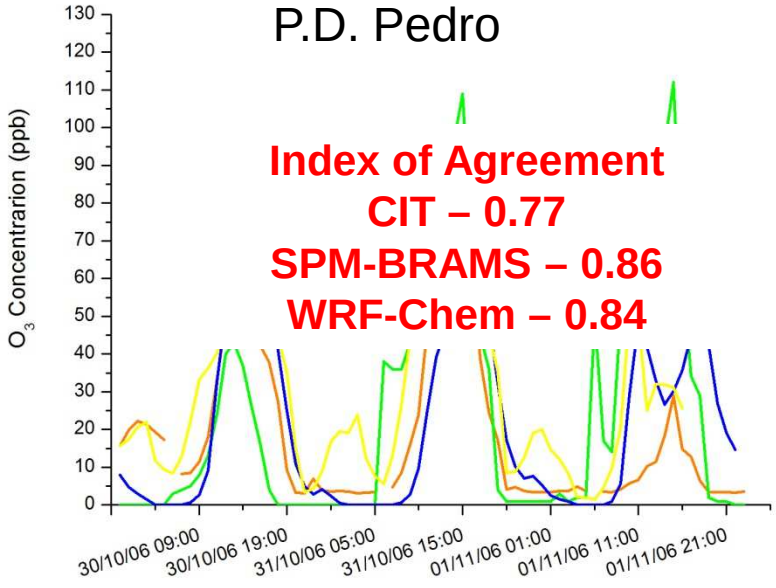
P.D. Pedro



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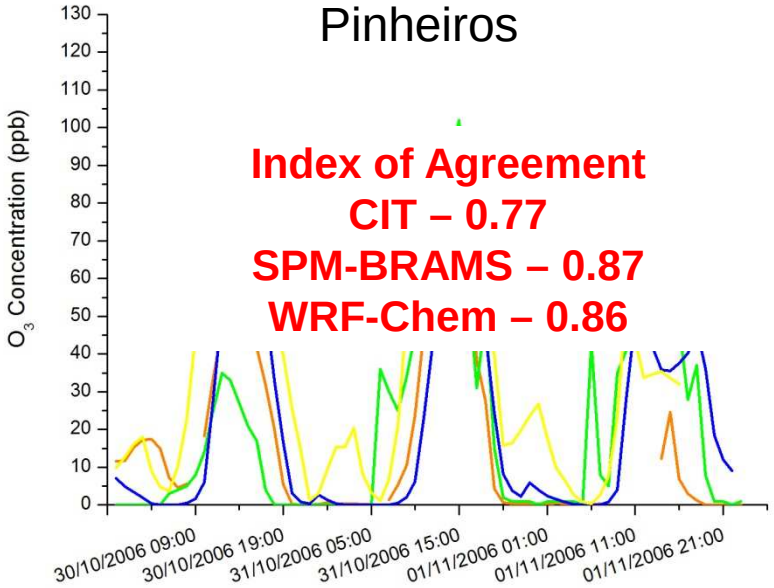

Index of Agreement
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SPM-BRAMS – 0.87
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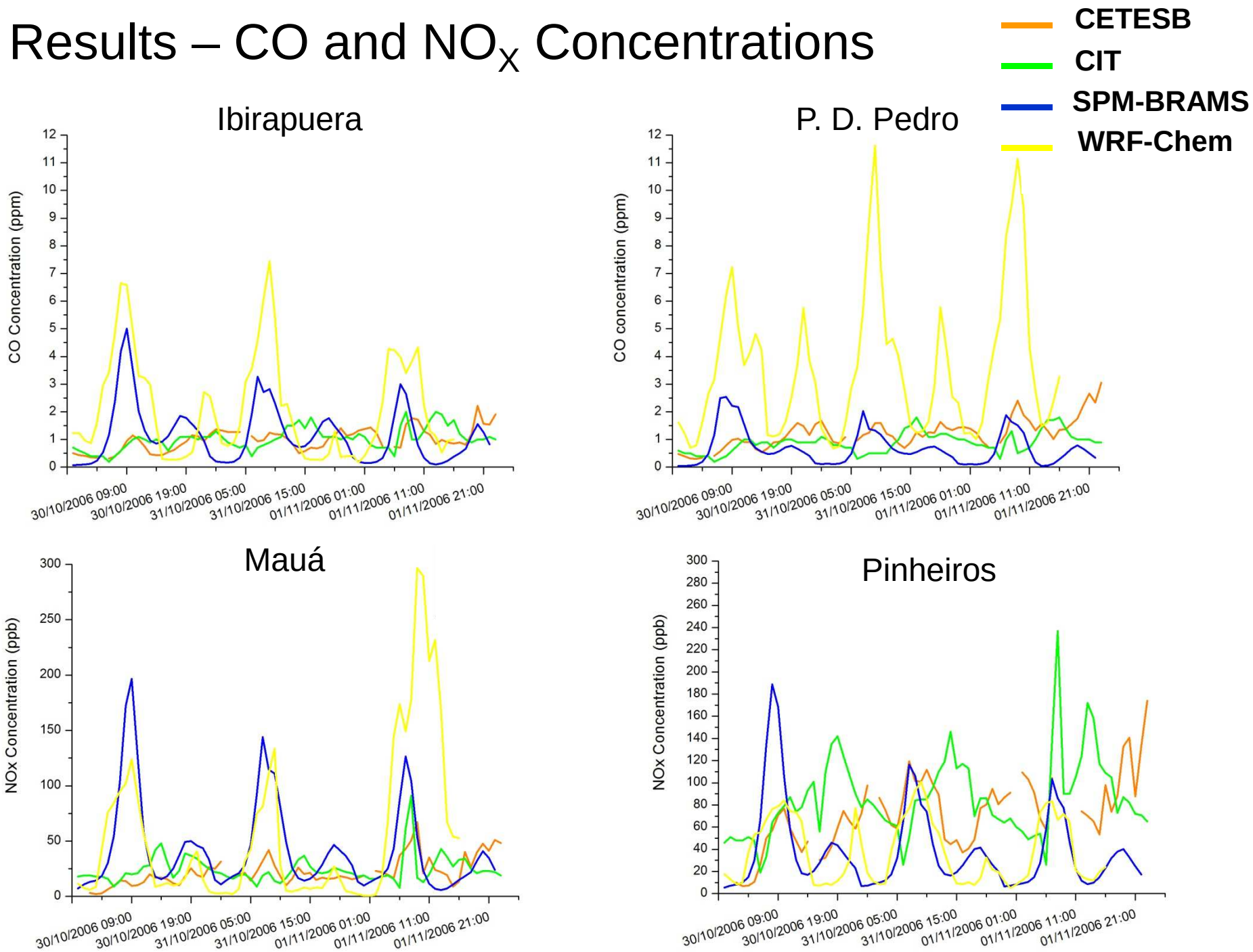
Results – CO and NO_X Concentrations



Summary

- Despite the simplified chemistry, the SPM-BRAMS shows good results when simulating the ozone concentrations, except when those had exceed the Brazilian NAAQS.
- In general, CIT and WRF-Chem registered values above of the observed ones and show a better performance to simulate higher ozone levels.
- CIT results did not represent well the abrupt concentration decrease during night-time and in the last campaign day.
- All three models had not registered good results simulating CO and NO_X concentrations. WRF and BRAMS results overestimated the concentrations values while CIT, in general, had results at the same magnitude order.

Summary

- One of the main problems concern the use of photochemical models in the MASP is the lack of a detailed atmospheric emissions inventory.
- In SPM-BRAMS, the chemical simplification of volatile organic compounds and the spatial distribution of the emissions in the region can be responsible for the results founded for CO and NOX concentrations.
- CIT presents problems with the inadequate representation of the surface and the use of interpolated hourly average meteorological data that impact the numerical representation of several meteorological processes that affect the air quality in the MASP.