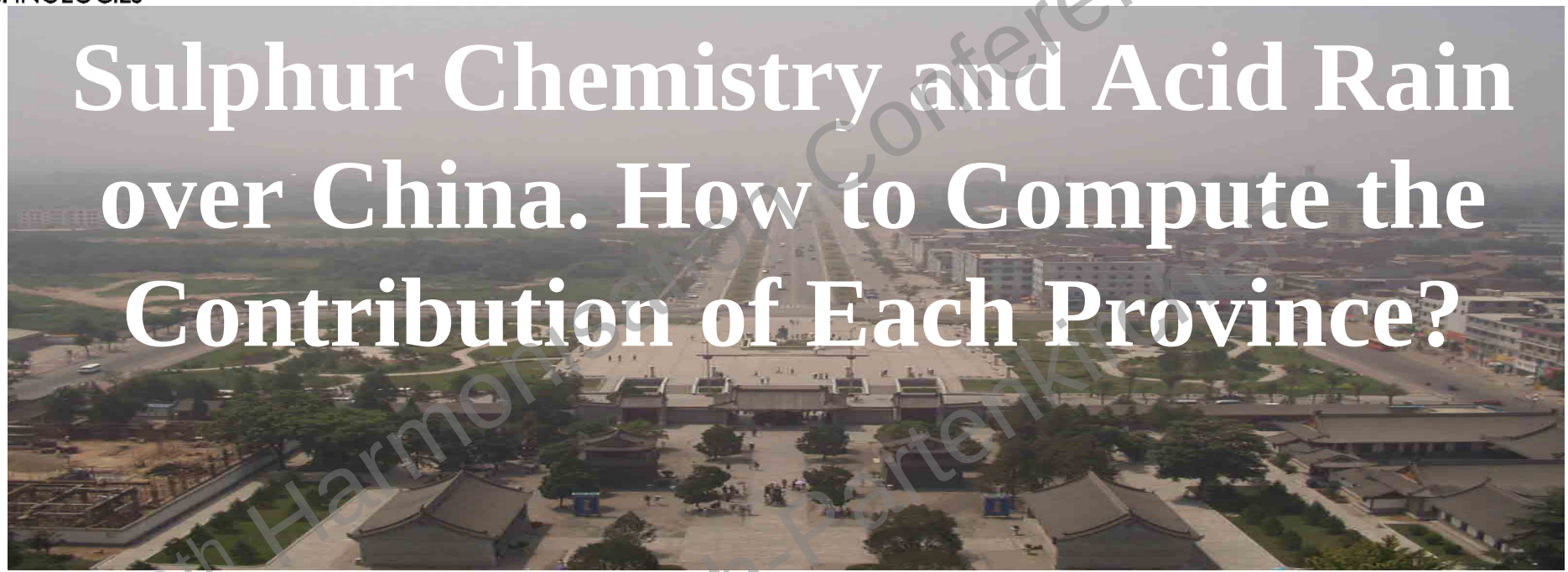
9th International Conference on Harmonization within Atmospheric Dispersion Modeling for Regulatory Purposes - June 2004

Sulphur Chemistry and Acid Rain over China. How to Compute the Contribution of Each Province?



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[1]China National Environmental Monitoring Center Beijing China
[2]ARIA Technologies SA Boulogne-Billancourt France
[3]Institut Pierre Simon Laplace CNRS France

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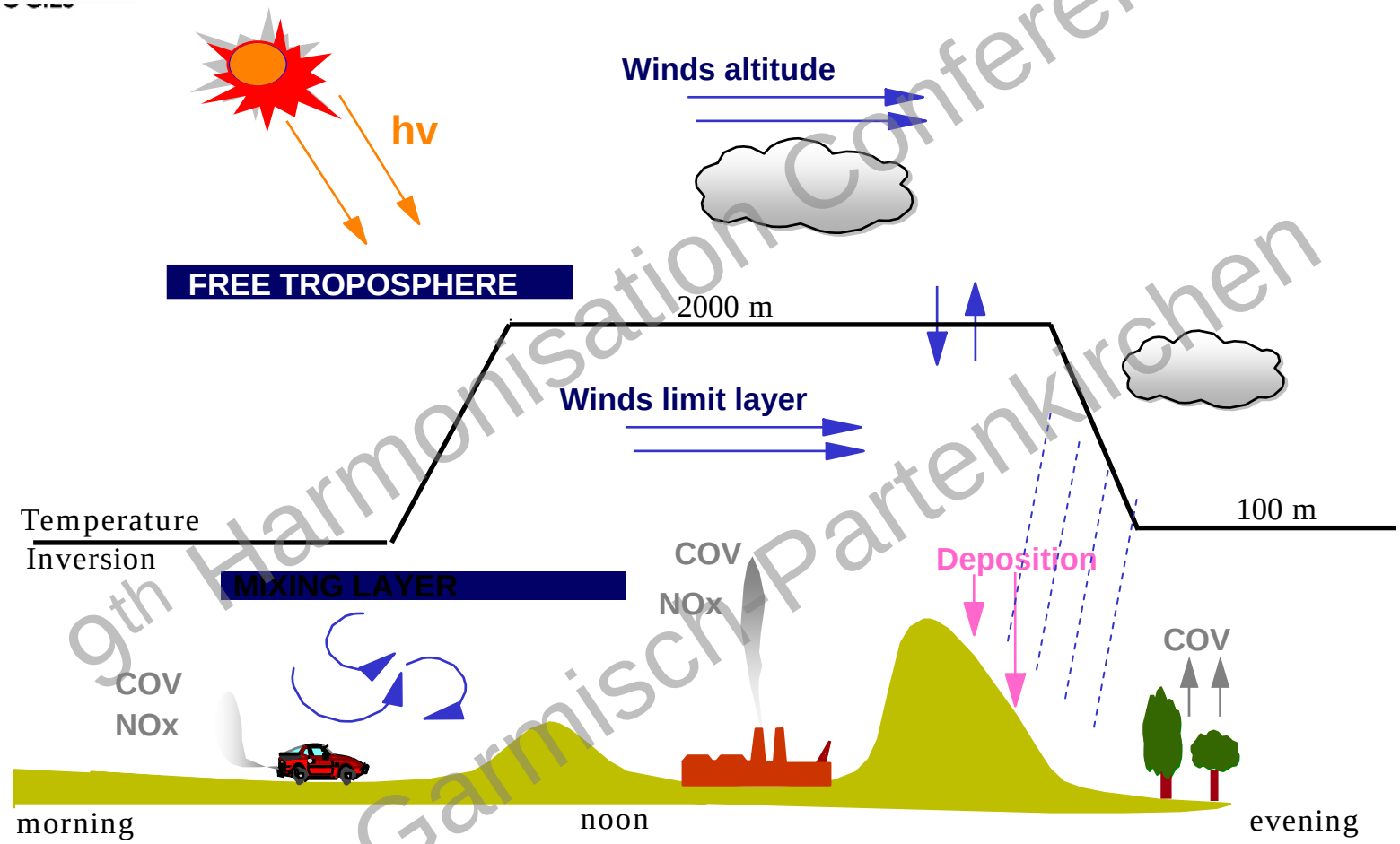
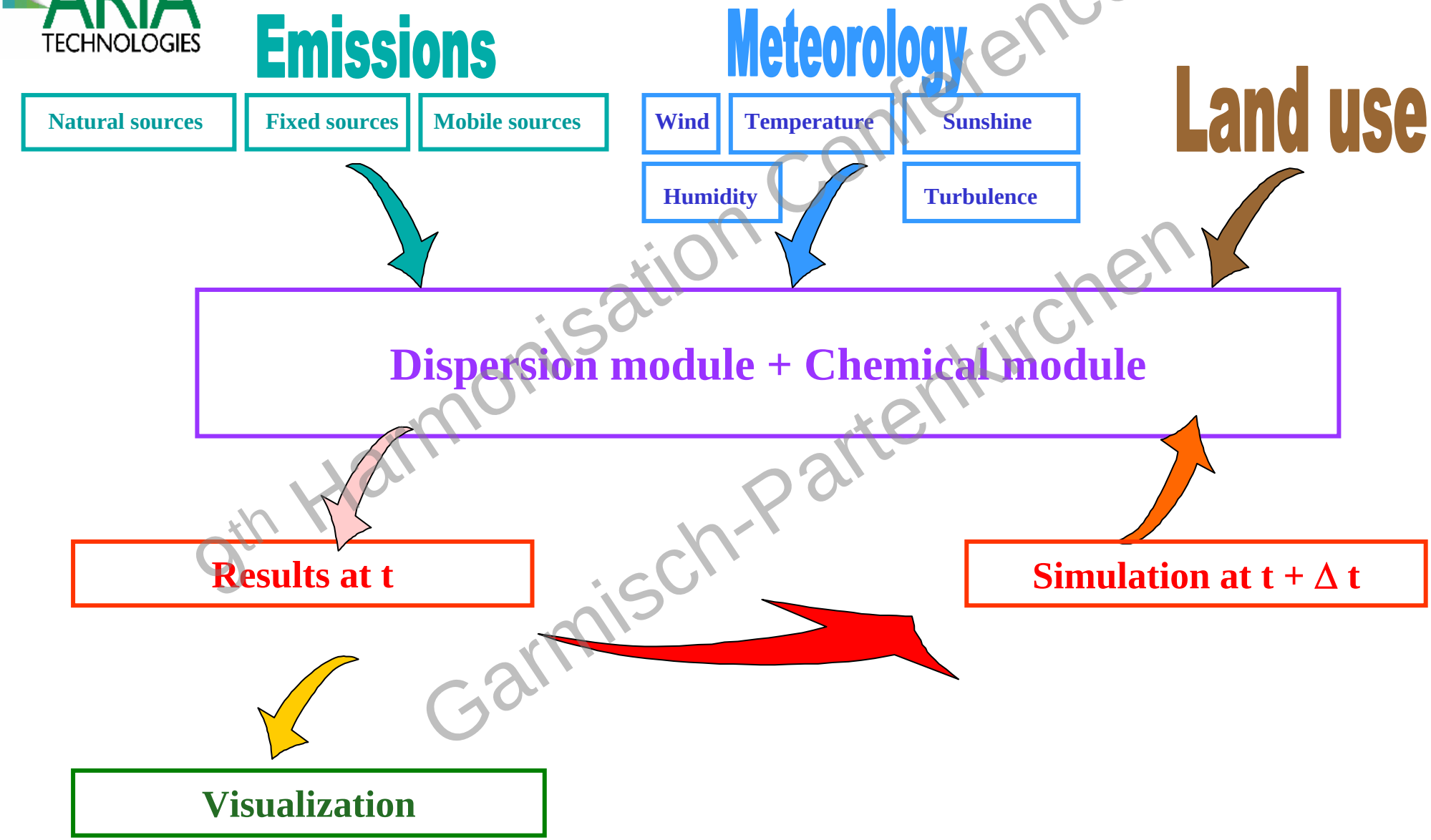
Summary

- ➔ Software « CHIMERE » at the CNEMC
  - (1) Acid rain at continental scale
  - (2) Transportation of desert dust
- ➔ One year modeling (Year 2000)
  - (1) Simplified version (Climatological values for O_3, OH, H_2O_2)
  - (2) With all photochemical reactions
- ➔ Comparison with CNEMC data
- ➔ Photo-oxidant pollutants
- ➔ Flux exchanges between provinces

Processes taken into account



Inputs Data Needed



Algorithms

- Chemical mechanism : adapted for SO_2 , H_2SO_4 gaseous and aqueous chemistry
  - Version 1.0 simplified (Climatologic ozone concentration)
  - Version 2.0 (with Ozone Chemistry : **48** species and **128** chemical reactions)
- Photolytic rate : attenuated by cloudiness
- Wet and dry deposition for SO_2 an H_2SO_4 :

  The Dry Deposition Velocity is calculated with a resistance approach as proposed by Wesely et al., (1989)

  In the case of the wet deposition, the following processes are considered :

  In-cloud scavenging of :

  - SO_4 aerosol
  - Gaseous species (now SO_2 and H_2O_2)

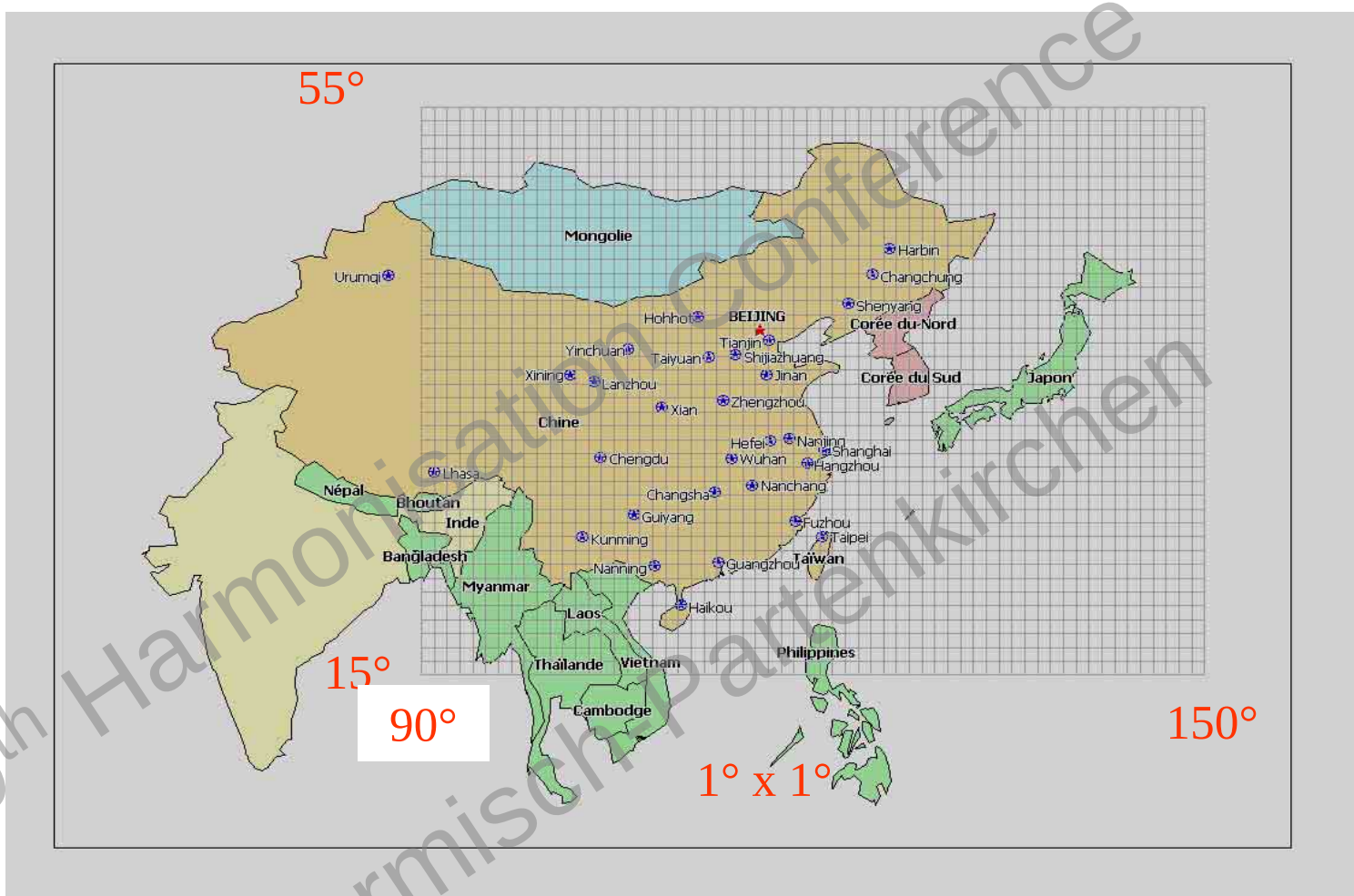
  Sub-cloud scavenging of :

  - SO_4 aerosol
  - Highly soluble gaseous species (now H_2O_2)
- Numerical time solver : TWOSTEP method

SOFTWARE

- Reactive dispersion model :
  - CHIMERE V1.0 programs, input and output files
- Scientific software :
  - NetCDF,
  - GMT
  - GSVIEW
- High performance visulization SAVI_3D software
- MeRAF Converter (Chimere➔SAVI_3D)

Showcase Grid



– Latitude : 15°N-55°N resolution 1° Longitude : 90°E-150°E resolution 1°

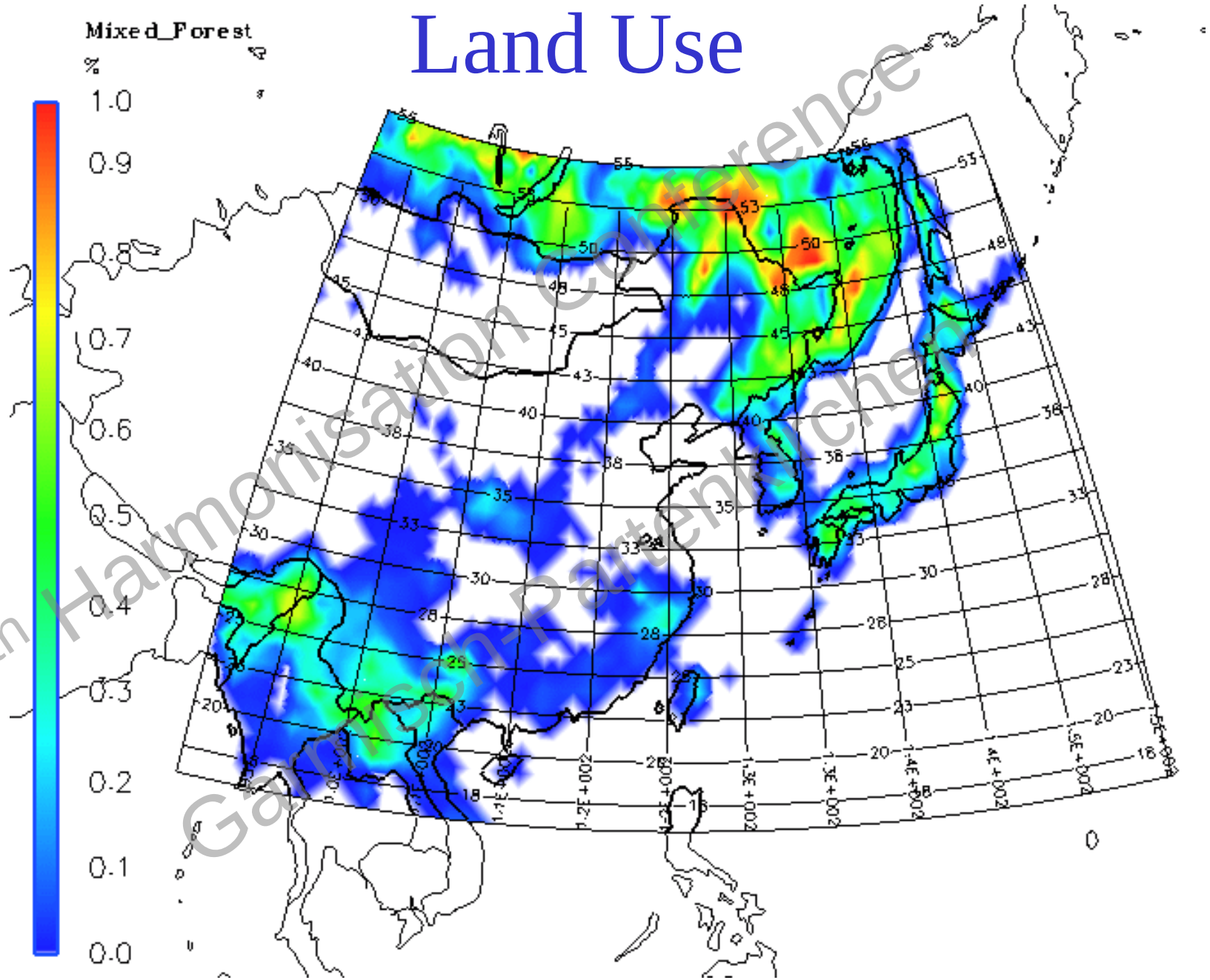
– 7 levels including the all PBL from surface to 400 hPa

– 60x40=2400 meshes x 7 levels

Input data

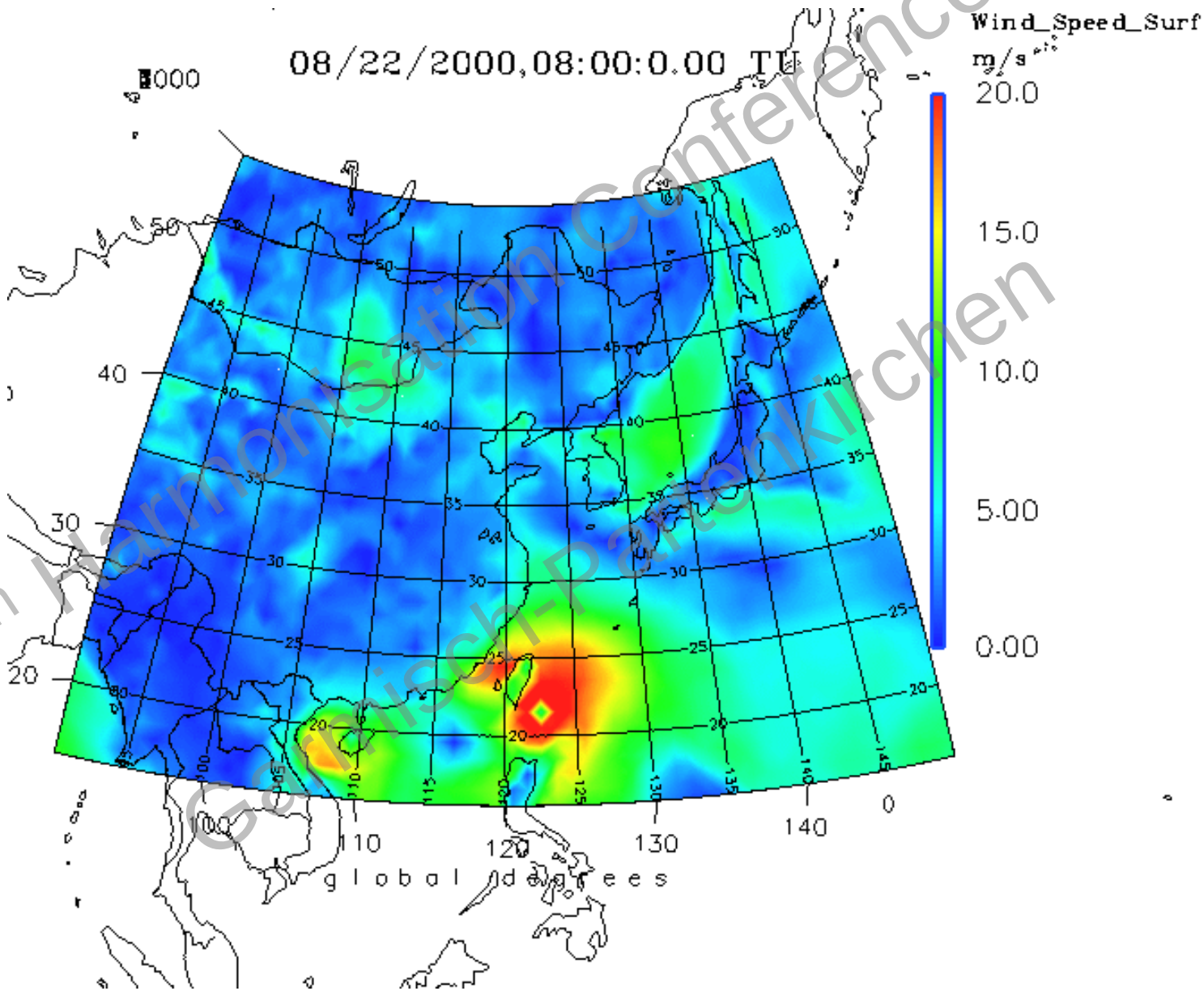
- Land Cover : USGS (U.S. Geological Survey)
  15 land use categories
- Topography : same as ECMWF
- Meteorology : ECMWF (Centre Européen de Prévisions météorologiques à moyen terme) Reading UK
- Emissions :
  - ACE-Asia (Asian Pacific Regional Aerosol Characterisation Experiment)
    - Y2000
    - resolution 1°x1° http ://saga.pmel.noaa.gov/aceasia
  - Seasonal modulation from GEIA (1985)

Land Use

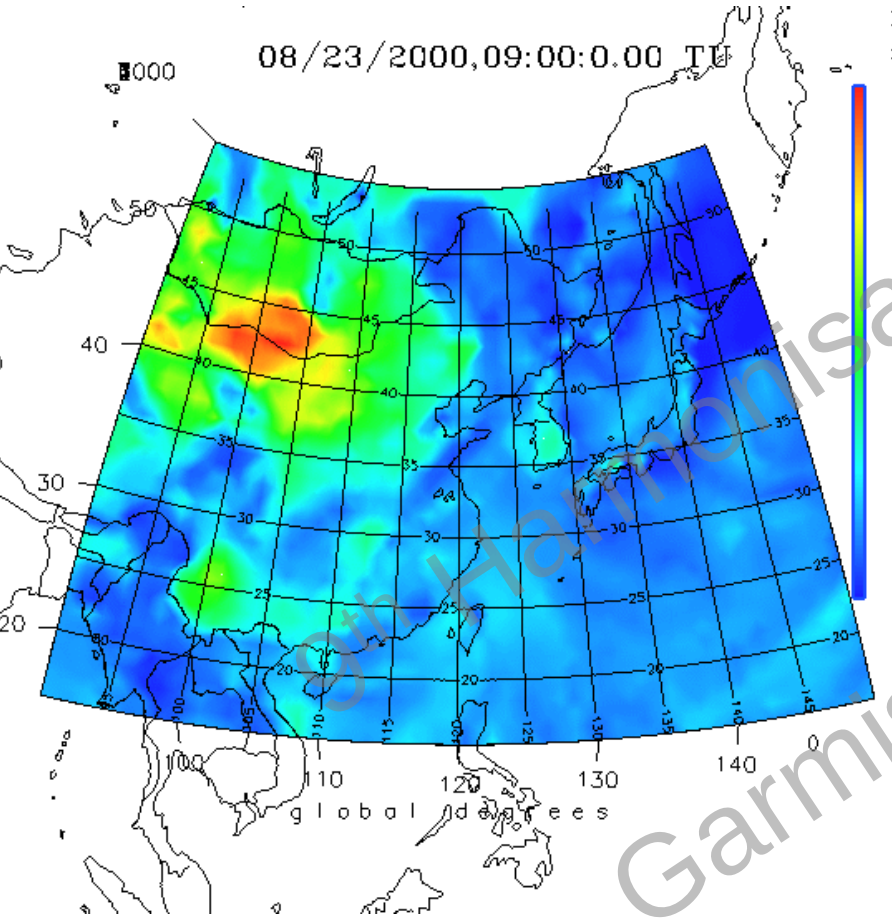


Test on a episode

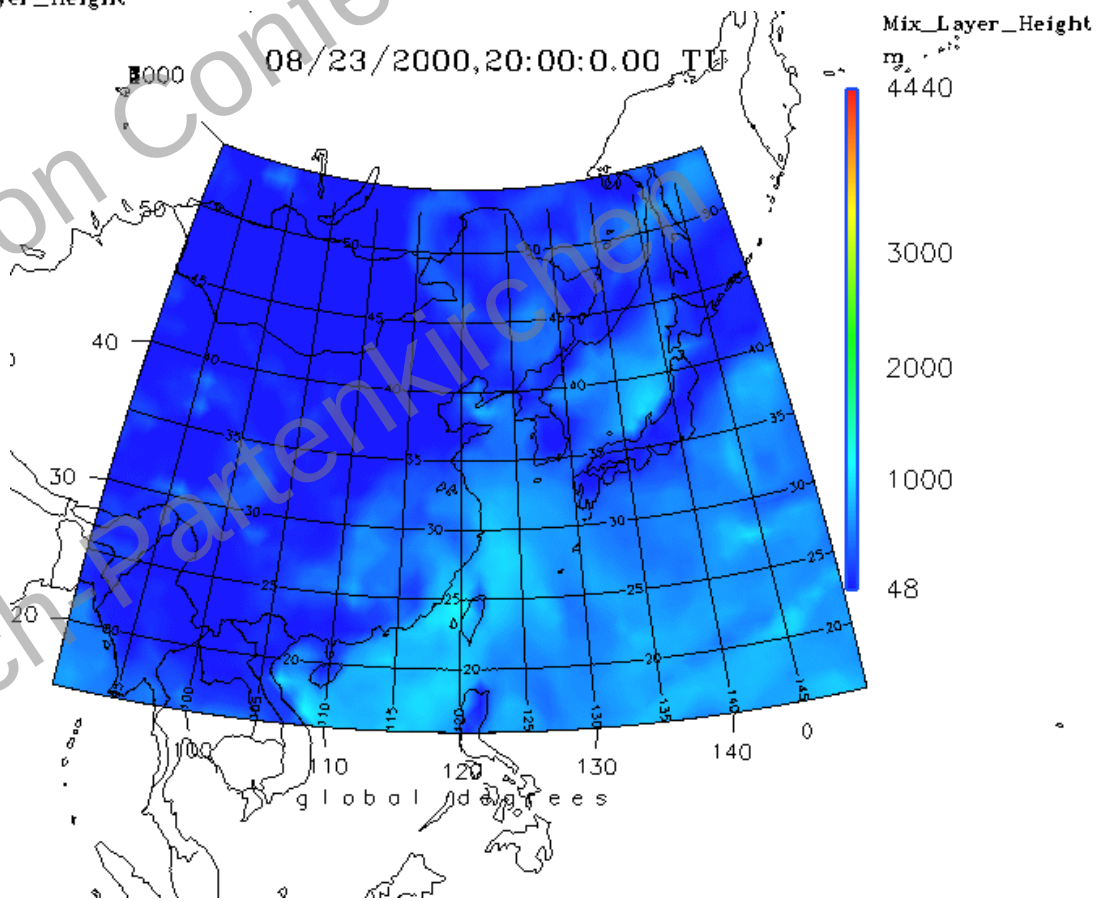
Surface wind



Mixing layer height

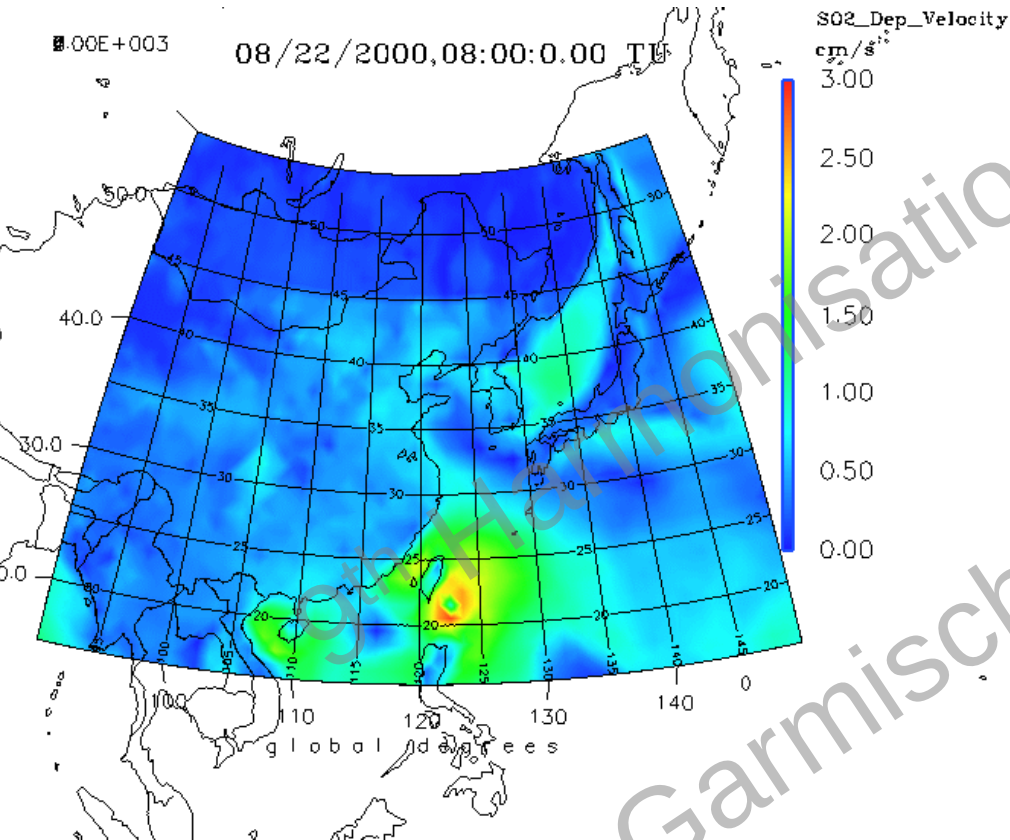


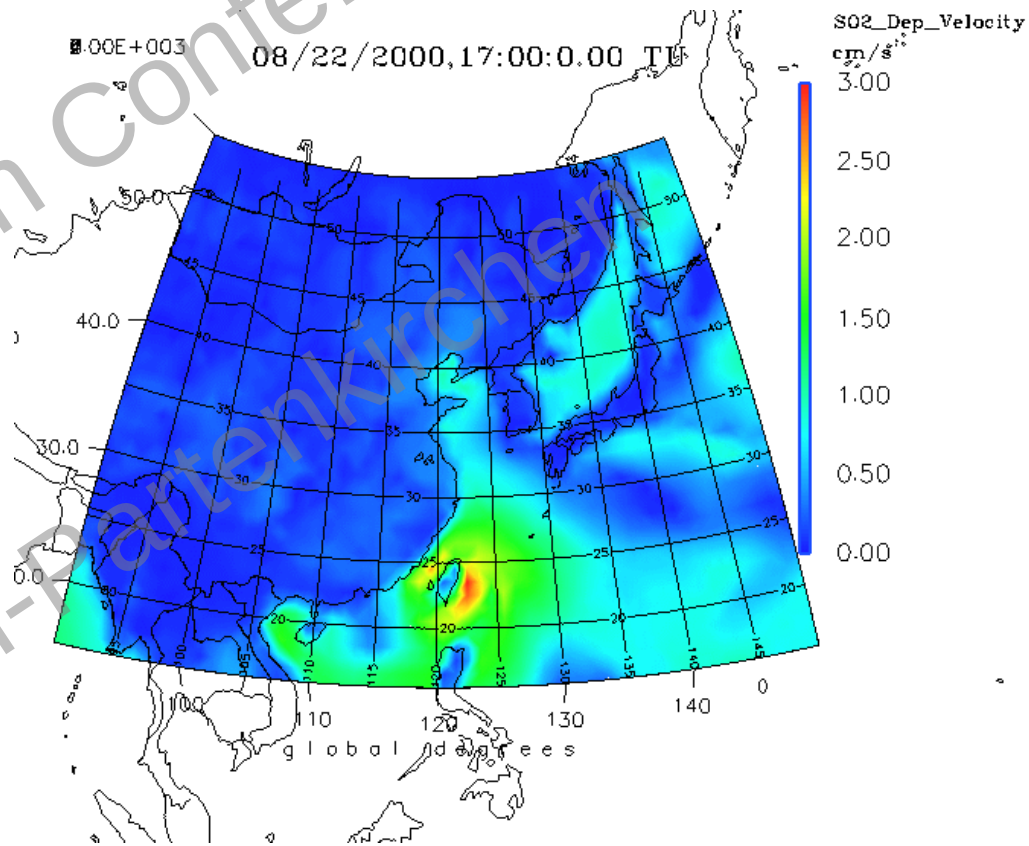
day



night

SO_2 dry deposition velocity

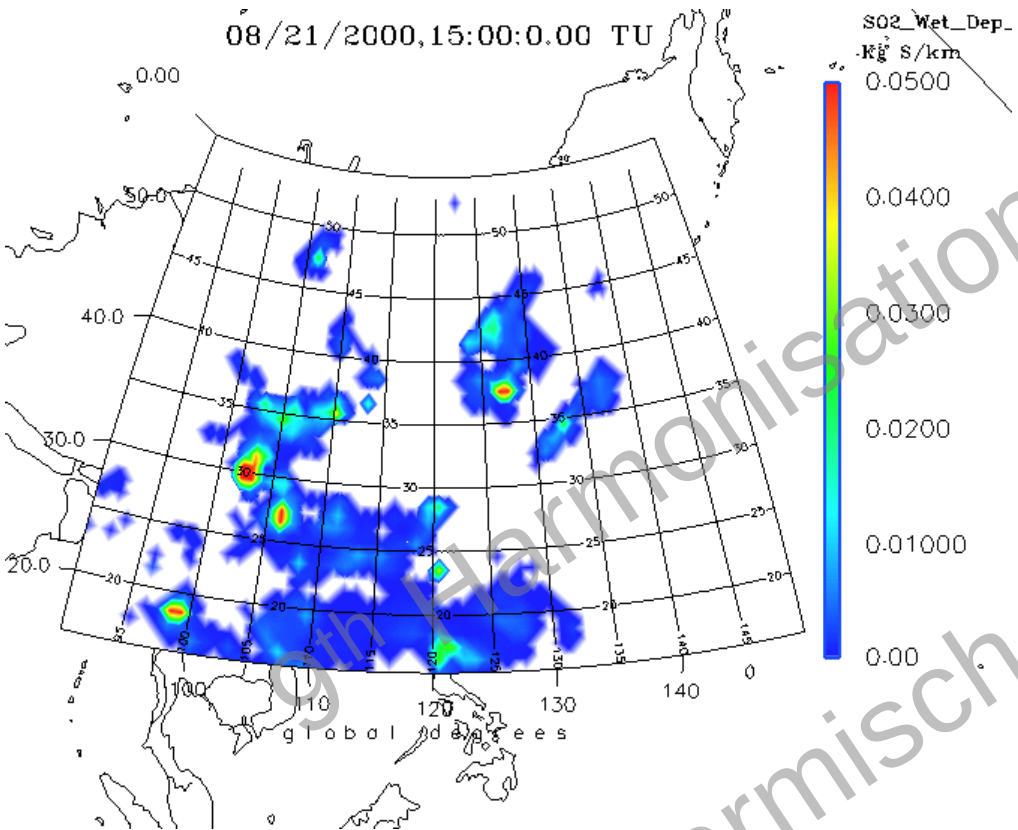


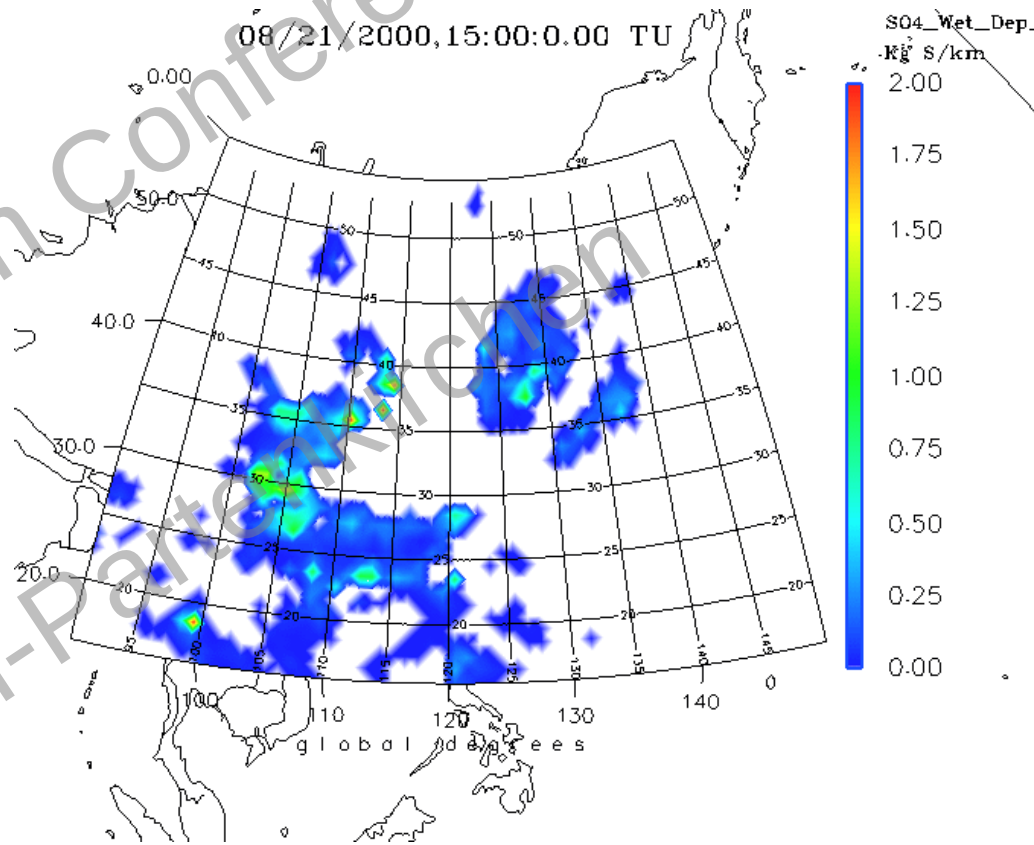


day

night

SO_2 wet deposition

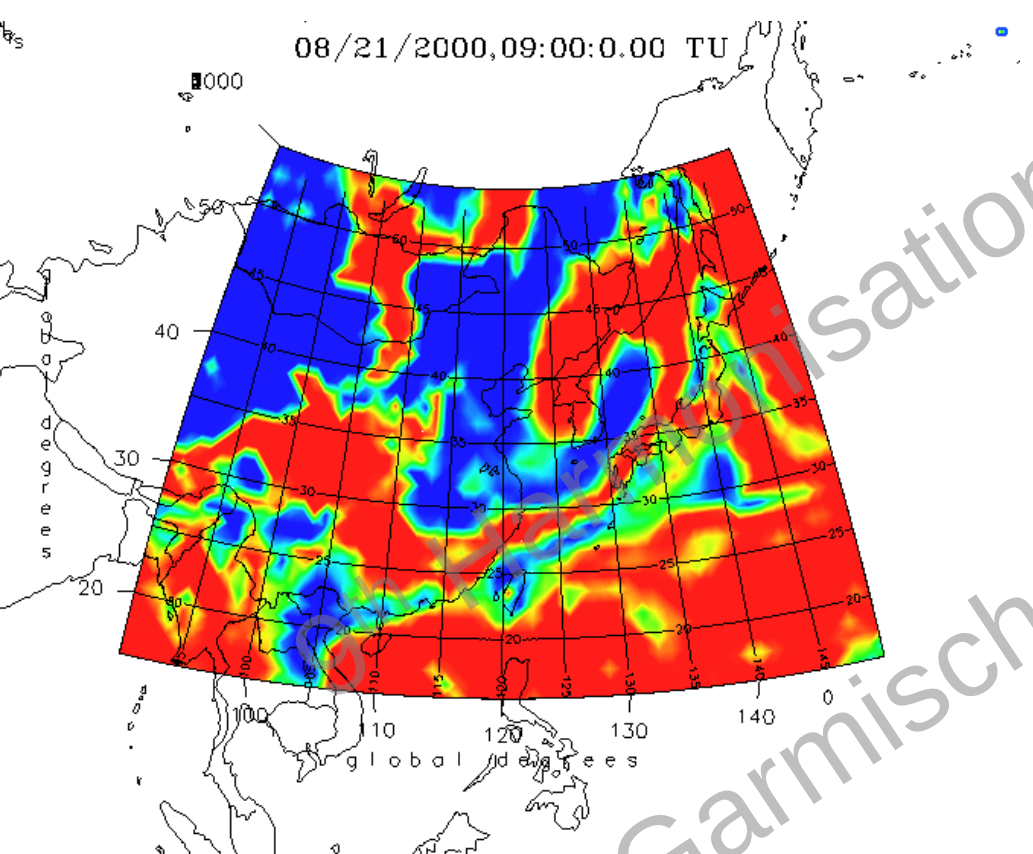


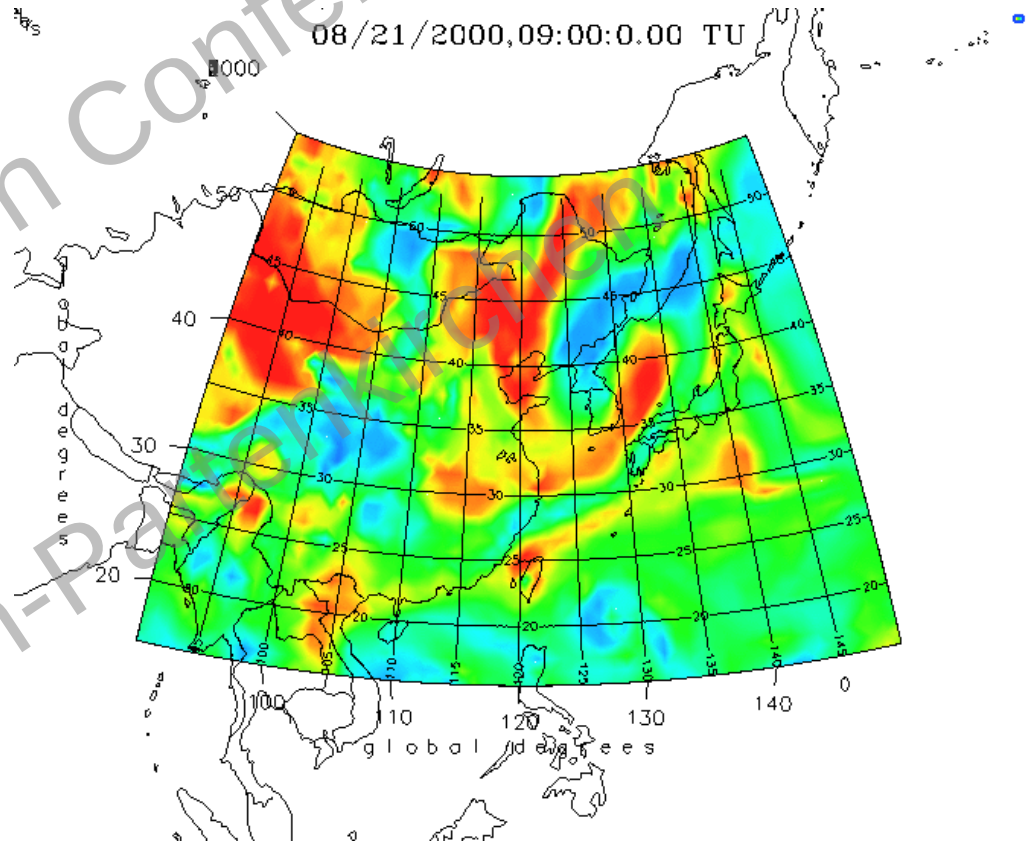


SO_2

H_2SO_4

Low cloud fraction and photolysis reduction

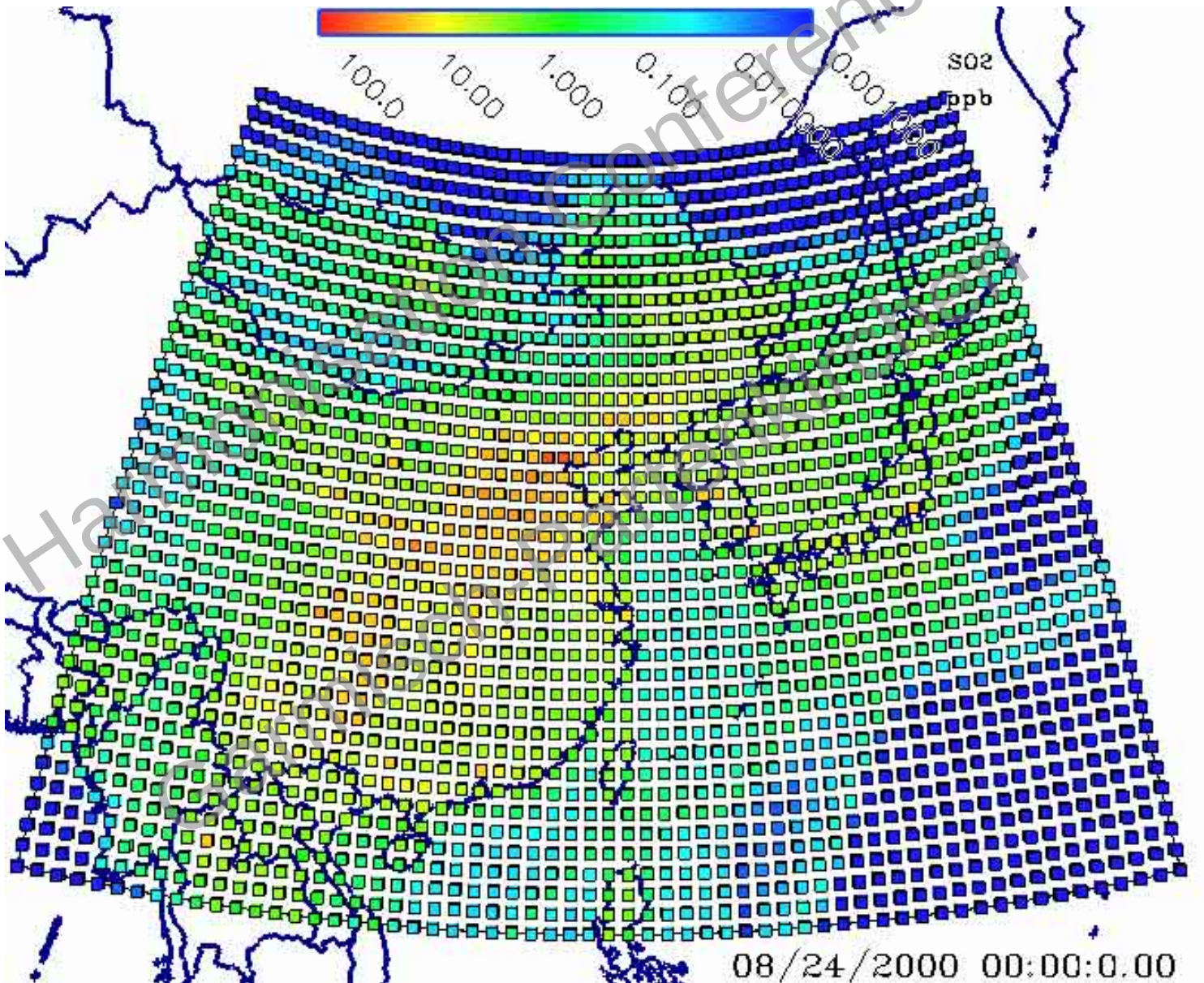




Low cloud cover

Photolysis reduction

Example of Episode



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➔ Comparison with CNEMC data

➔ Photo-oxidant pollutants

➔ Flux exchanges between provinces

Yellow sand transport Episode

Yellow sand transport

3 days simulation

Yellow sand transport

3 days simulation

- Isosurface : 5ppb
- Z-Strecht×300

Yellow sand transport

- Transport including dry and wet deposition➔ OK
- To be completed / improved :
  - Source term evaluation linked with local meteorology
  - Chemistry including dust reaction
    - basic➔ acid neutralization

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Y2000 data collection
Emissions

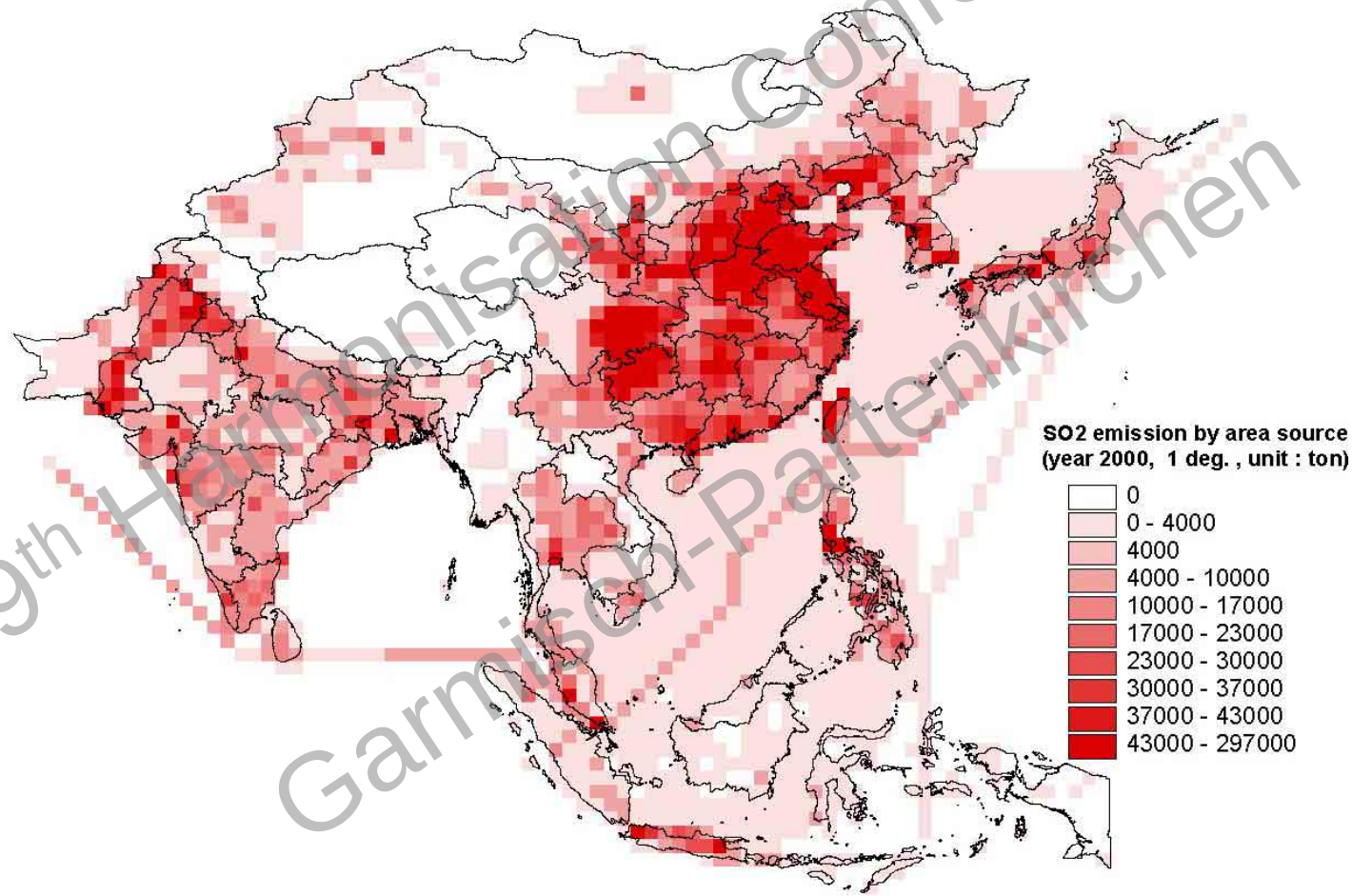
Pollution by activity type and Season modulation

	Industry	Housing	Transportation	Heat
SO2	35 %	14 %	2 %	49 %
NOx	23 %	8 %	42 %	27 %
VOCs	30 %	36 %	33 %	1 %
CO	14 %	10 %	34 %	42 %

No seasonal modulation (industry and transportation)

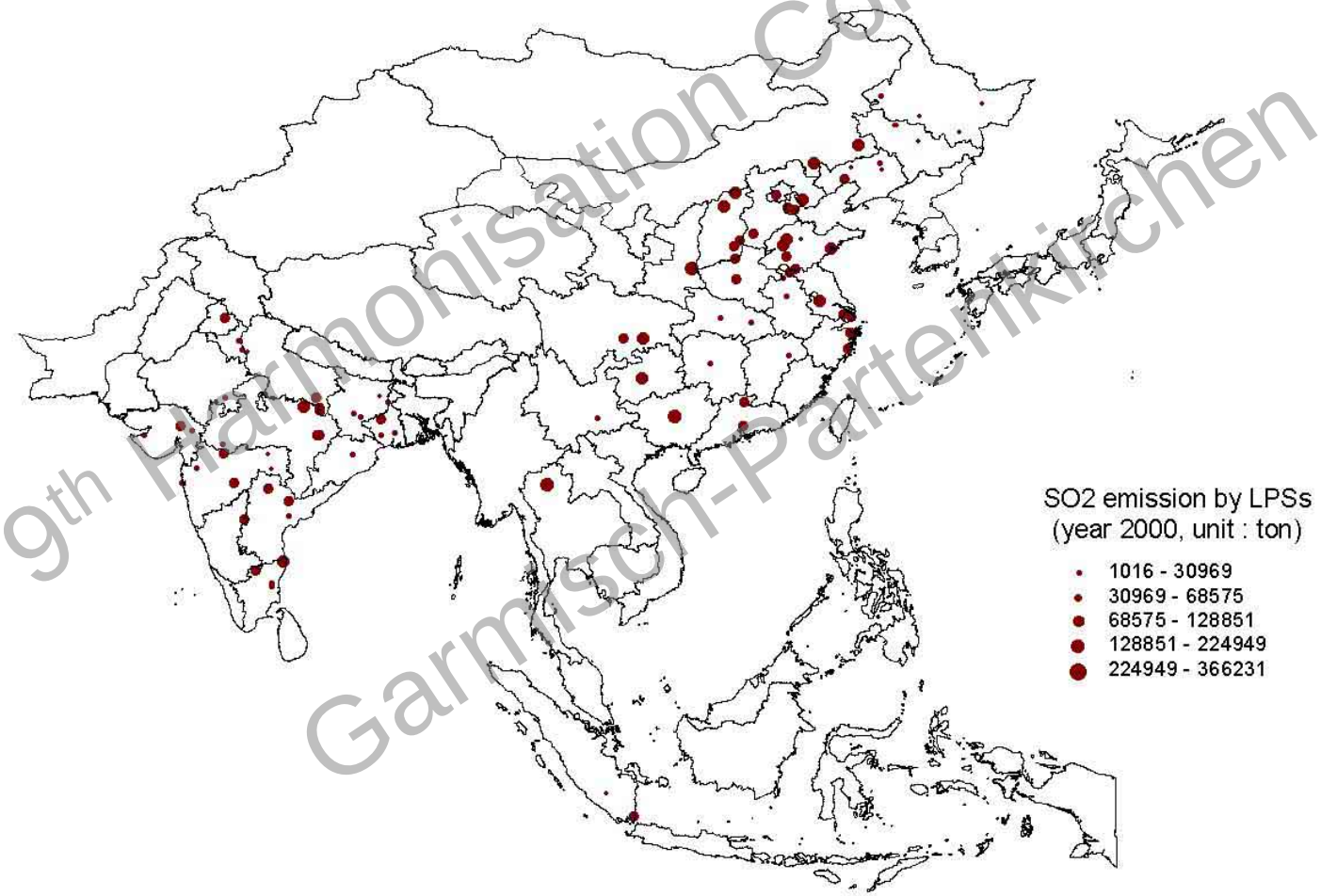
Seasonal modulation as SO2 (GEIA - 1985)

ACE-Asia
SO_2 area emissions

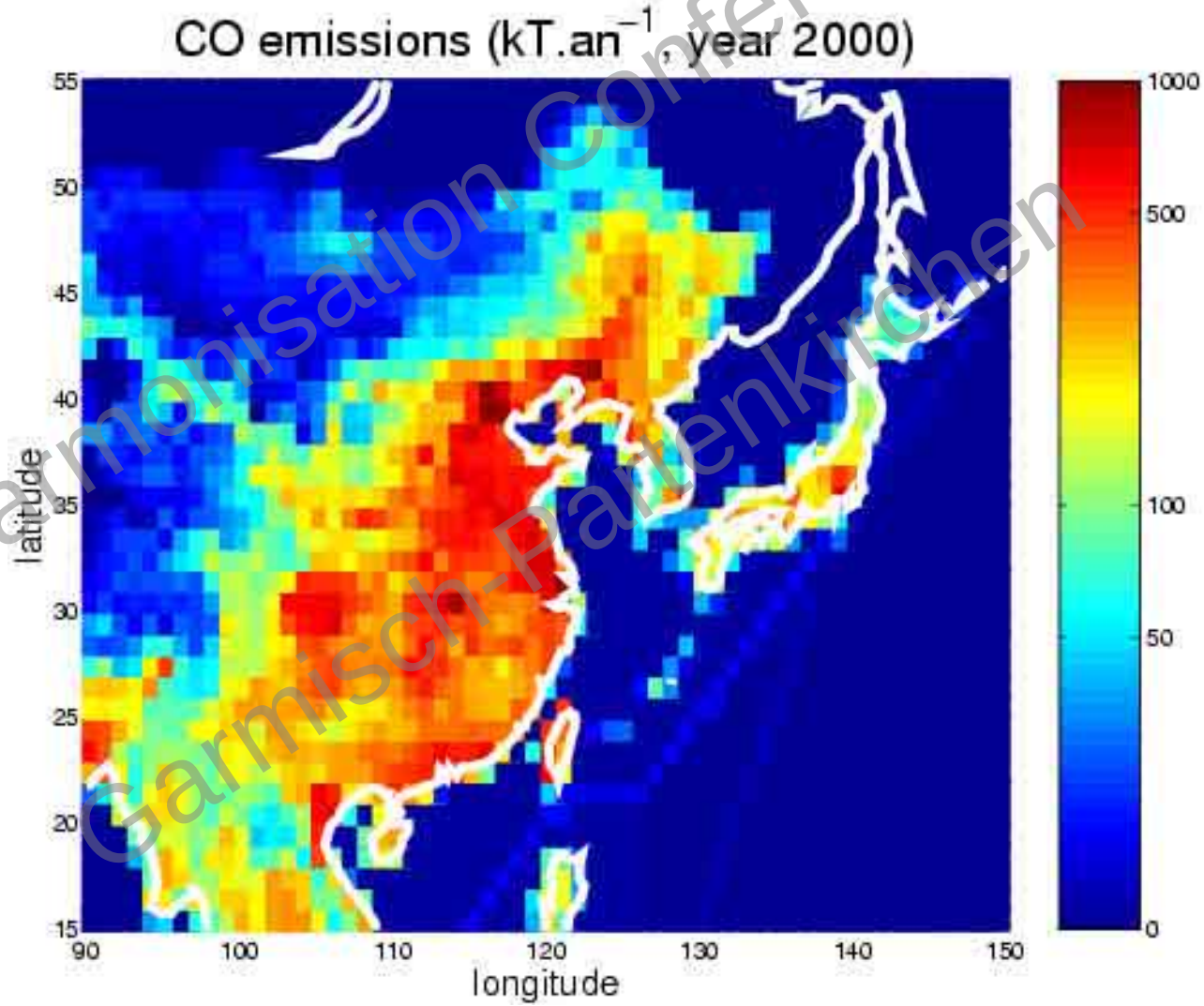


ACE-Asia

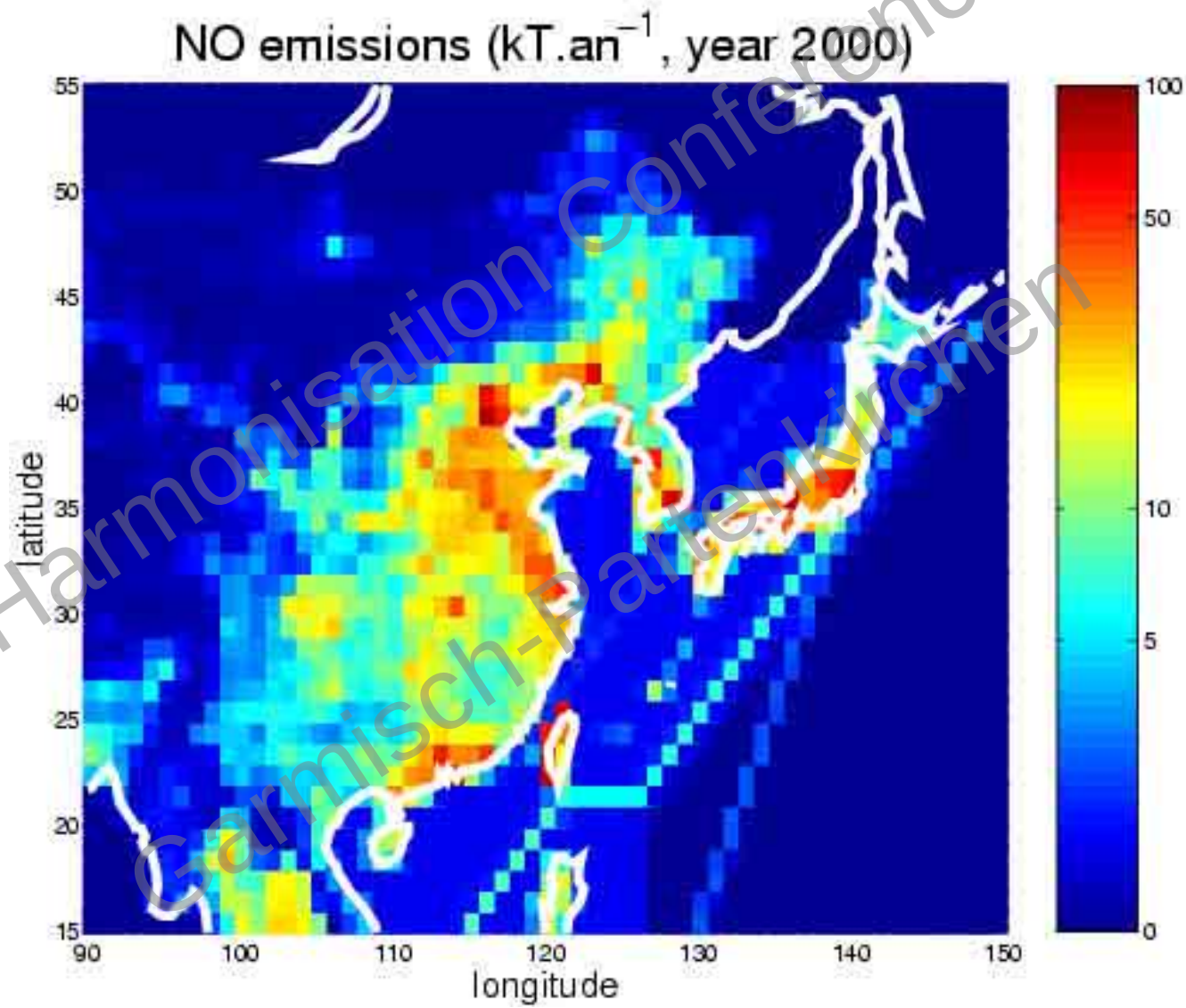
SO_2 large point sources emissions



CO emissions



NO emissions



VOC Speciation

Correspondance between VOC Klimont et al (2002) and MELCHIOR VOC

Spéciation de Klimont et al (2002)	Espèces contenues dans MELCHIOR
Ethane	Ethane
Propane	n-butane
Butane	n-butane
Autres alcanes	n-butane
Ethène	Ethène
Propène	Propène
Autres alcènes	Propène
Acétylène	½ Propène + ½ n-butane
Benzène	O-xylène
Toluène	O-xylène
Autres aromatiques	O-xylène
Formaldéhyde	Formaldéhyde
Autres aldéhydes	Acétaldéhyde
Cétone	Butan-2-one
Halocarbones	Non-réactifs
Autres COVs	n-butane

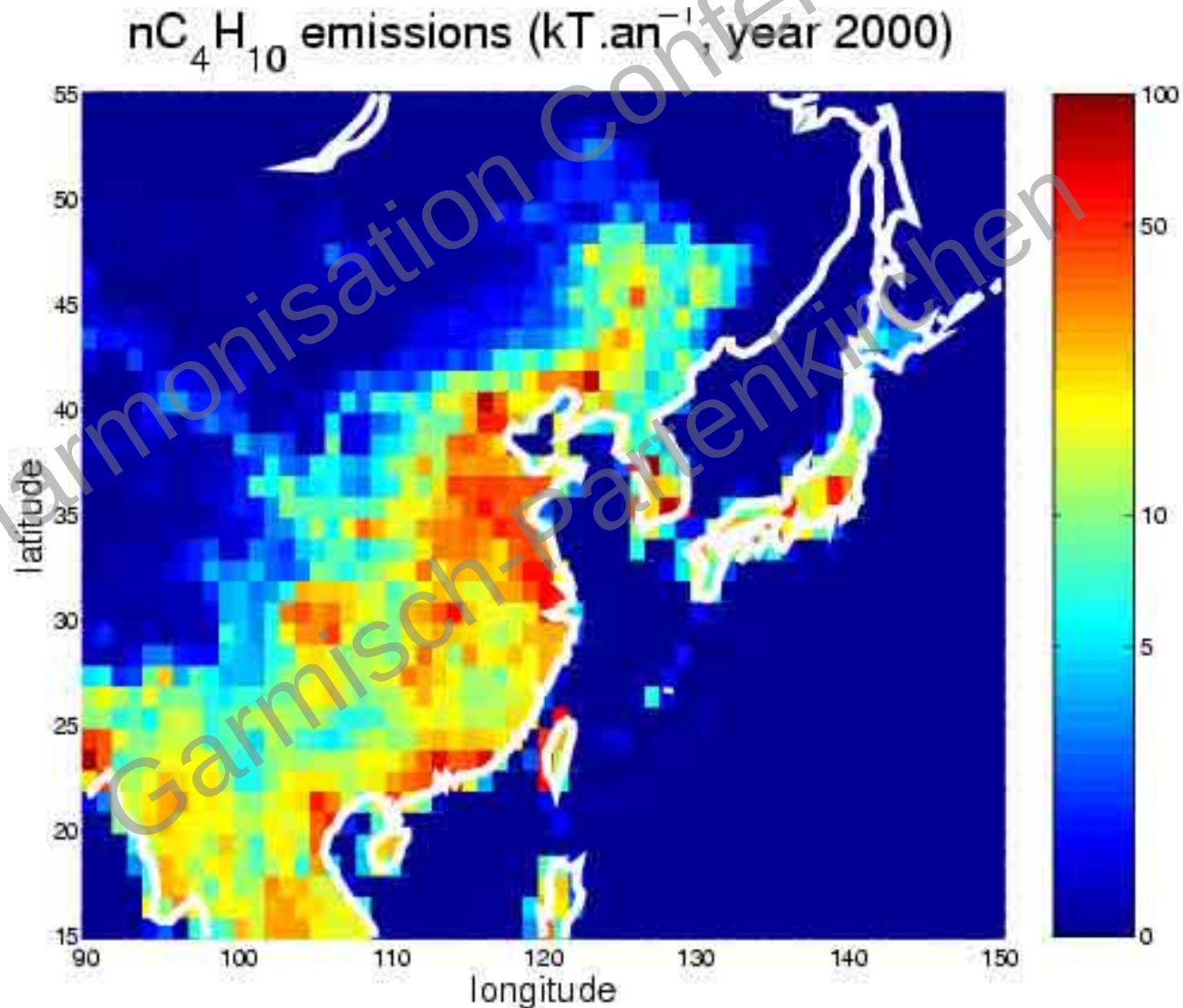
CHINA VOC speciation

COV dans MELCHIOR	Spéciation
Ethane	5.9 %
N-butane	41.1 %
Ethène	11 %
Propène	14.5 %
O-xylène	22.4 %
Formaldéhyde	1.1 %
Acétaldéhyde	1.8 %
Butan-2-one	1 %

Europe VOC

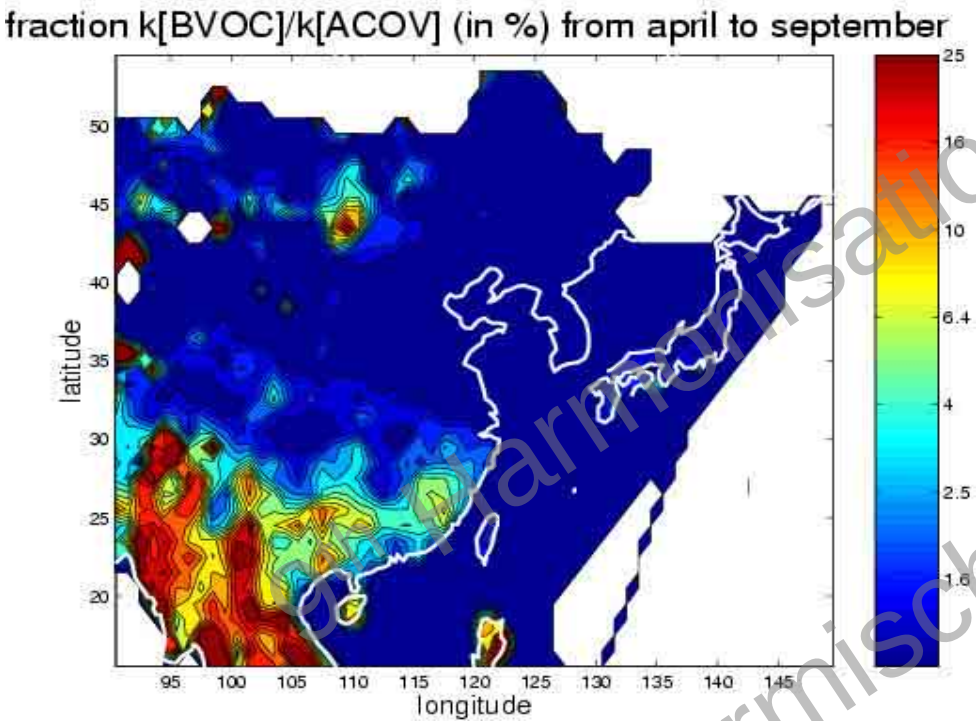
COV dans MELCHIOR	Spéciation
Ethane	26.3 %
N-butane	35.6 %
Ethène	7.1 %
Propène	15.6 %
O-xylène	6.6 %
Formaldéhyde	1.3 %
Acétaldéhyde	5.9 %
Butan-2-one	1.3 %

VOC emissions with speciation

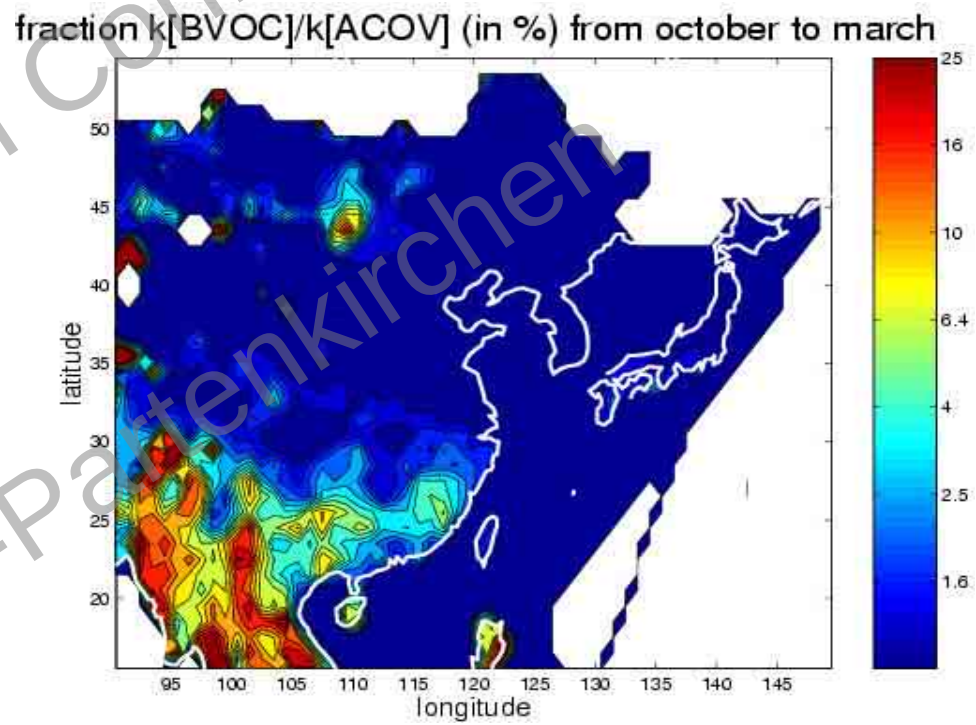


Ratio VOC Biogenic / Anthropogenic

- **Summer**



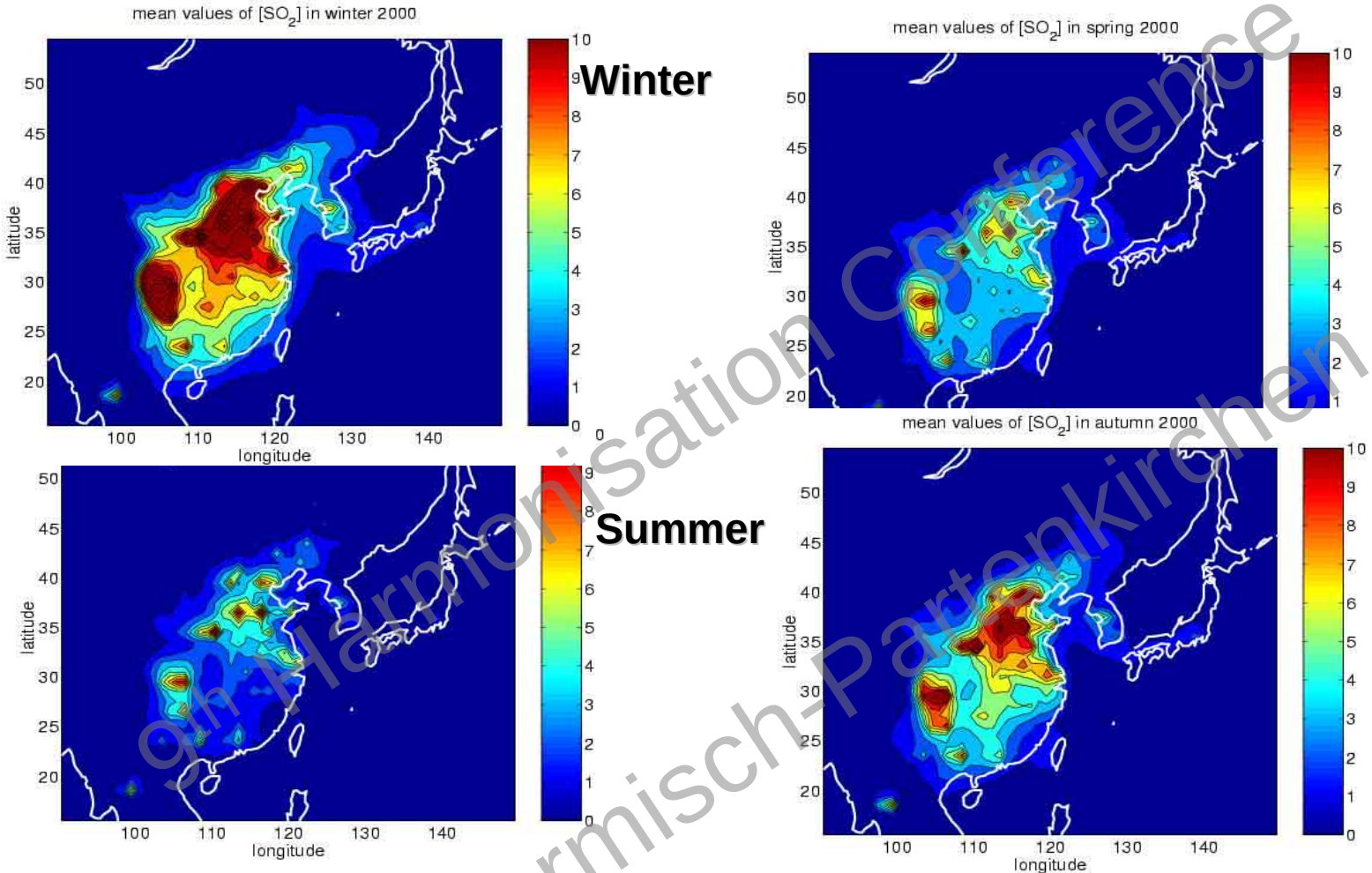
- **Winter**



➔ **Biogenic VOC emission are significant in the south**

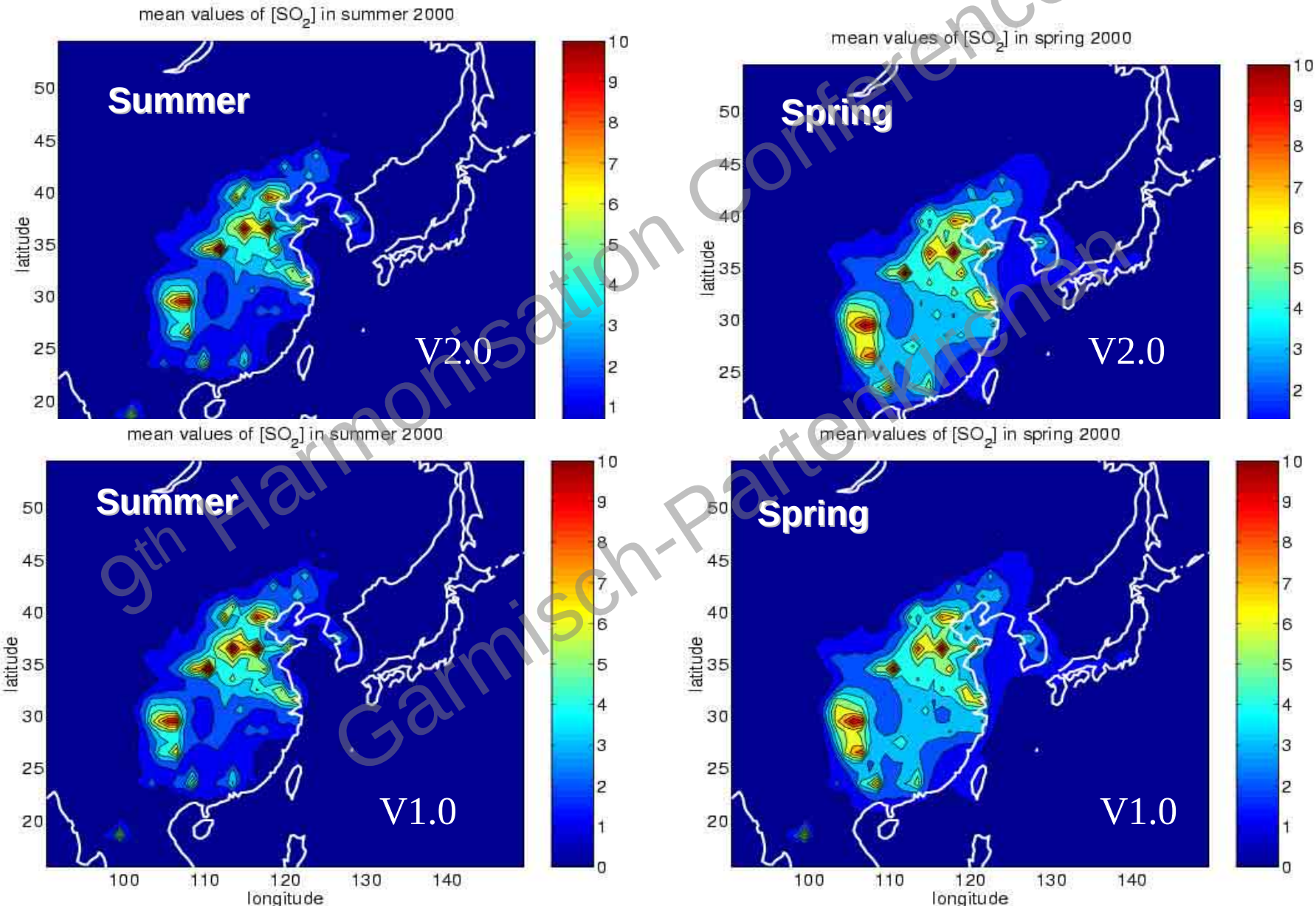
Main results (Year 2000)

Season Cycle on SO_2

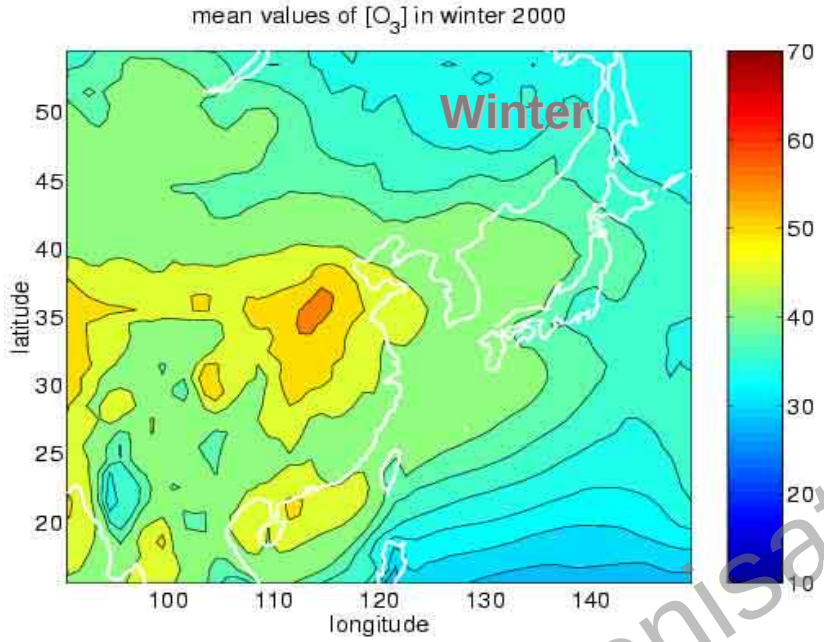


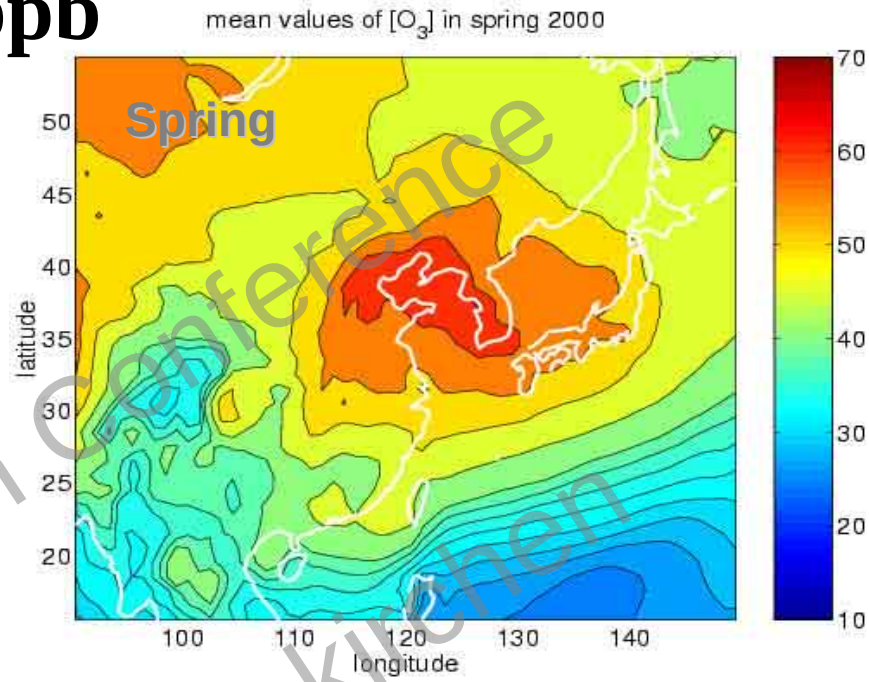
- **Mean [SO2] at 15 h TU lors de:**
  - **Winter (D,J,F)** **Spring (M,A,M)**
  - **Summer (J,J,A)** **Autumn (S,O,N)**
- **CHIMERE-chine 2.0**

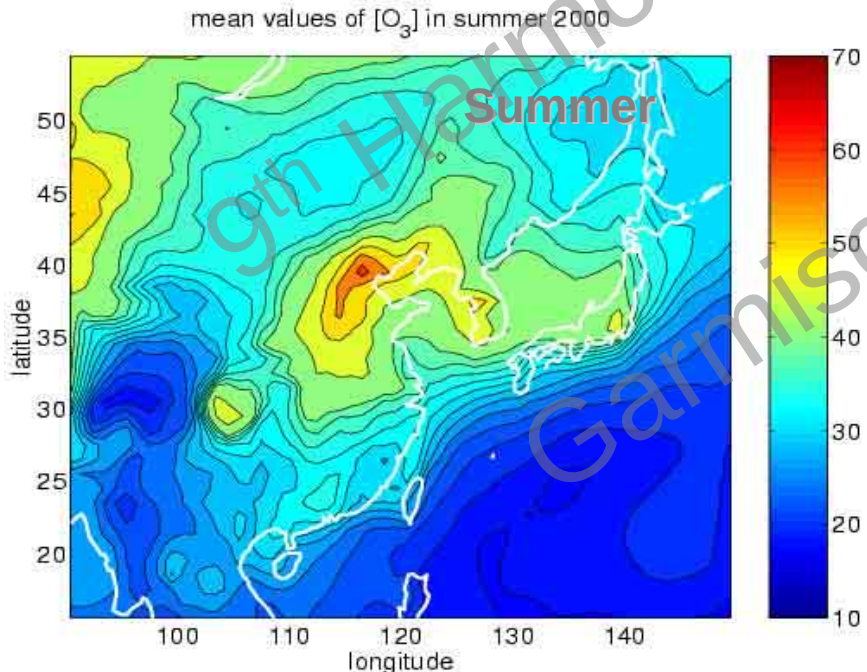
[SO2] comparison
CHIMERE-CHINE 1.0 et 2.0

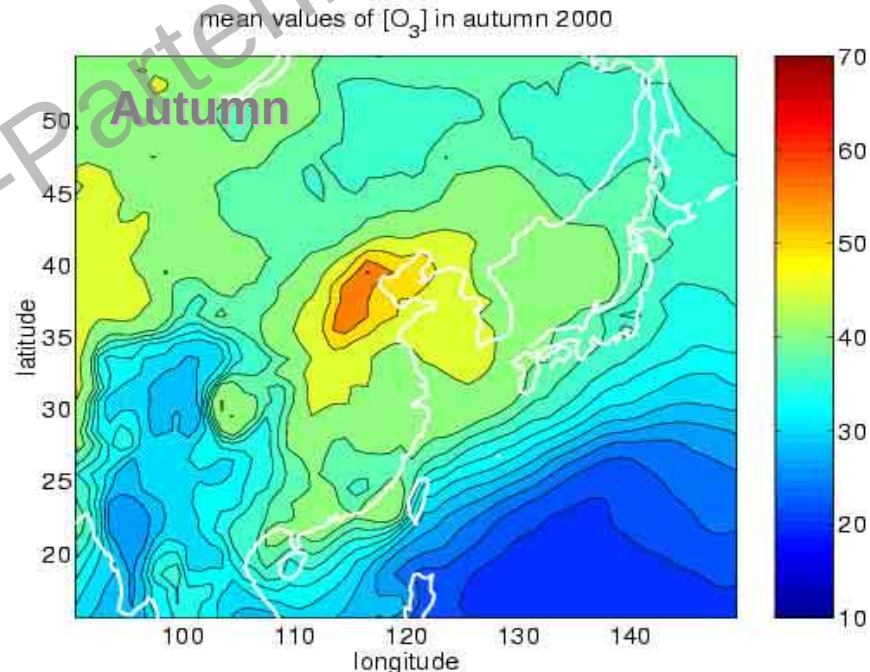


OZONE ppb





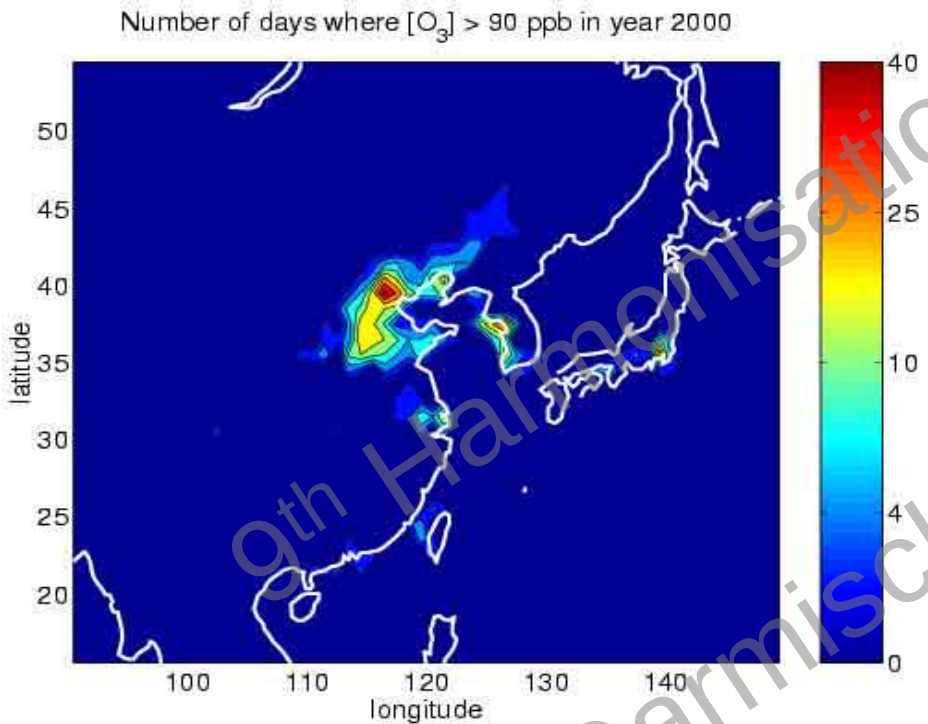




OZONE CONCLUSION

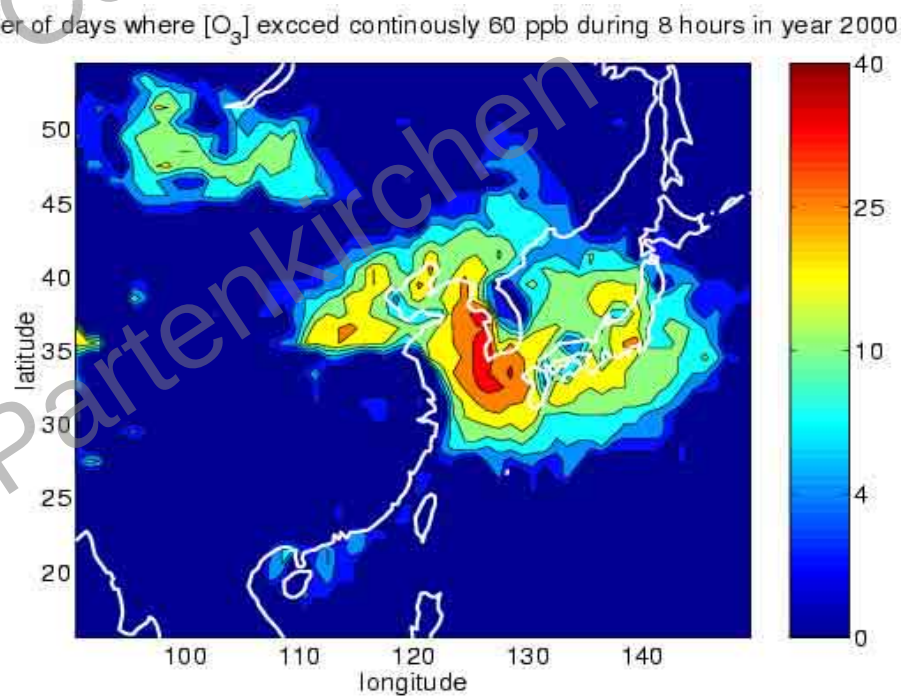
Number of days of threshold exceeded

UE value for public info ([O_3] > 90 ppb)



Number of days of threshold exceeded

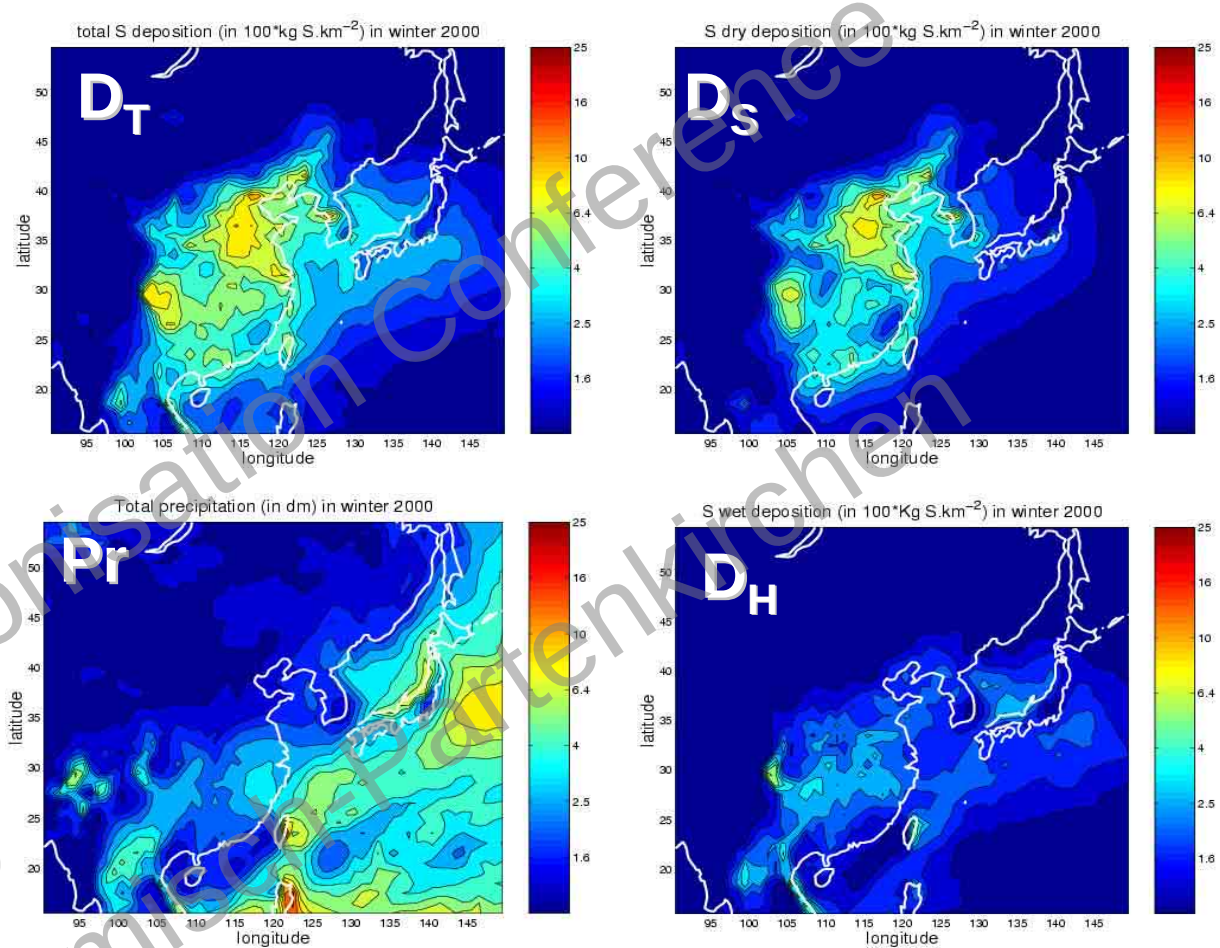
Mean 8h concentration > 60 ppb (public health recommandation)



➔ **Ozone policy needed mostly for the North part**

WINTER Sulfur deposition

- Cumulated deposition
- total (D_T),
- dry (D_S)
- wet (D_H))
- précipitations (Pr)
- Winter (D,J,F).
- CHIMERE-chine 2.0

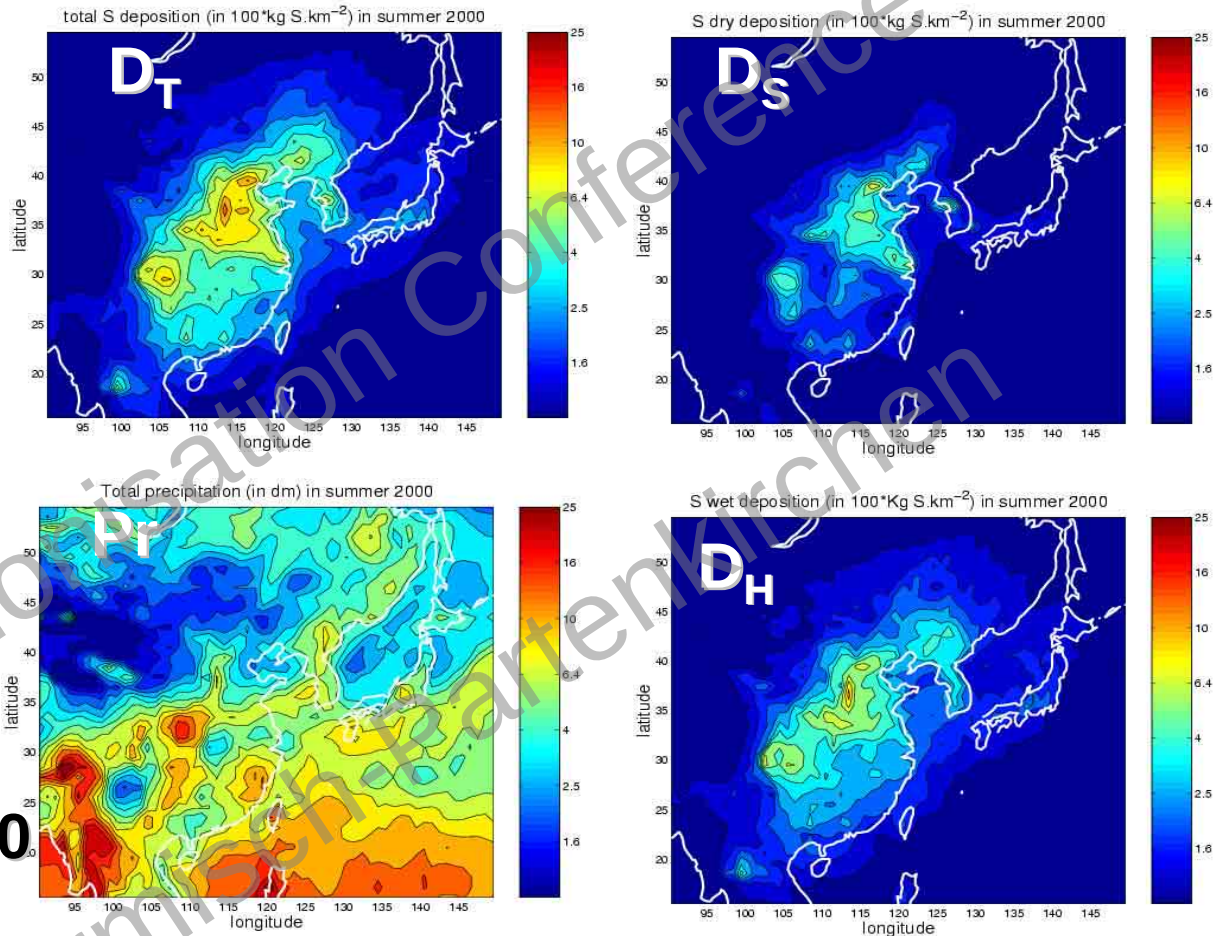


➔ Dry deposition mostly

➔ West to East transfer

SUMMER Sulfur deposition

- **Cumulated deposition**
- **total (D_T),**
- **dry (D_S)**
- **wet (D_H)**
- **precipitations (Pr)**
- **Winter (D,J,F).**
- **CHIMERE-chine 2.0**



➔ **Wet deposition more efficient**

Evaluation using CNEMC data (Year 2000)

Evaluation using CNEMC data

1. **50 ground station measurements SO_2 et de NO2 Hourly base 1 June 2000 → 31 december 2000.**
2. **Rain episode : measurements of H2SO4 and of the rainfall amount**

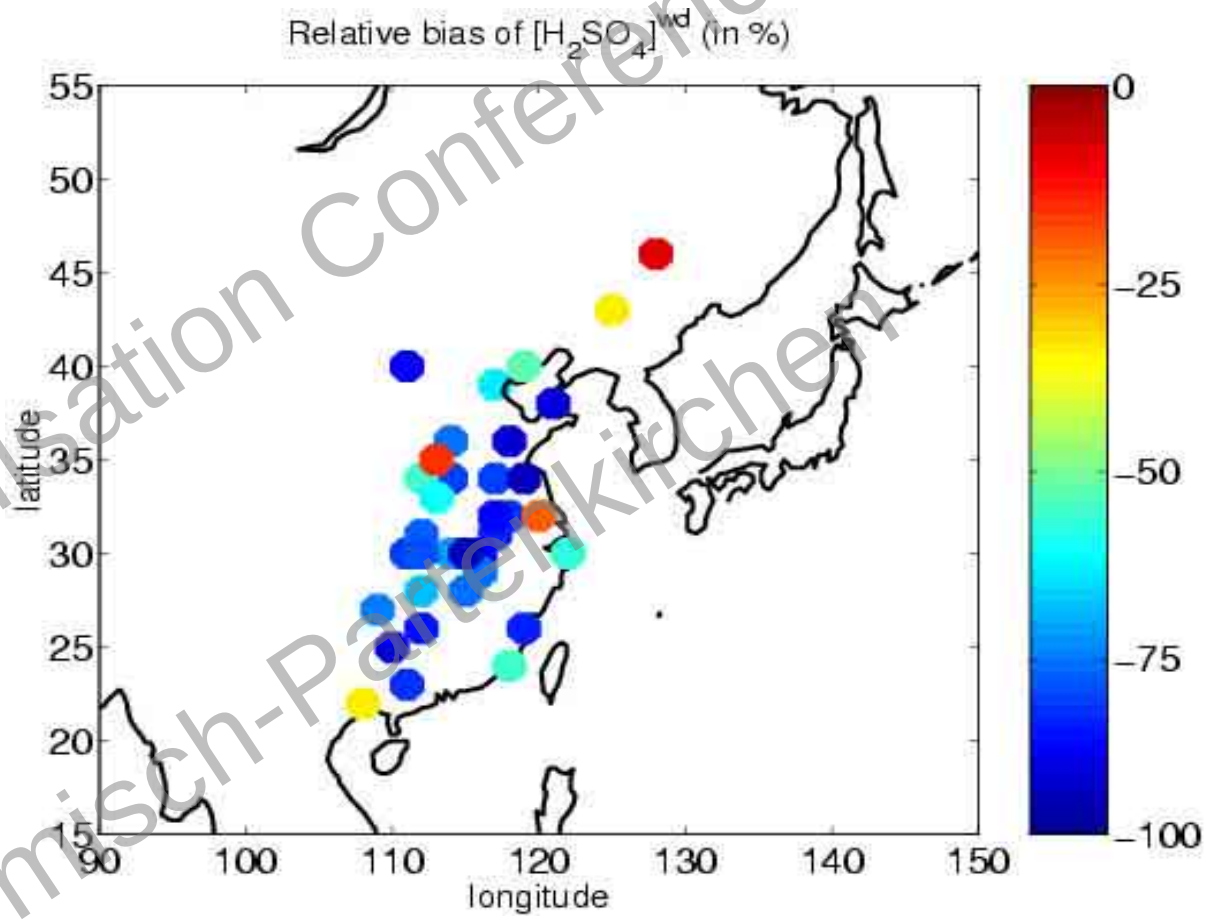
Note:

The evaluation is realized with CHIMERE-China version 2.0

[SO4] bias

- **1200 « episodes » over 54 sites.**

$$\frac{[H_2SO_4]_{mesure} - [H_2SO_4]_{modèle}}{[H_2SO_4]_{mesure}}$$

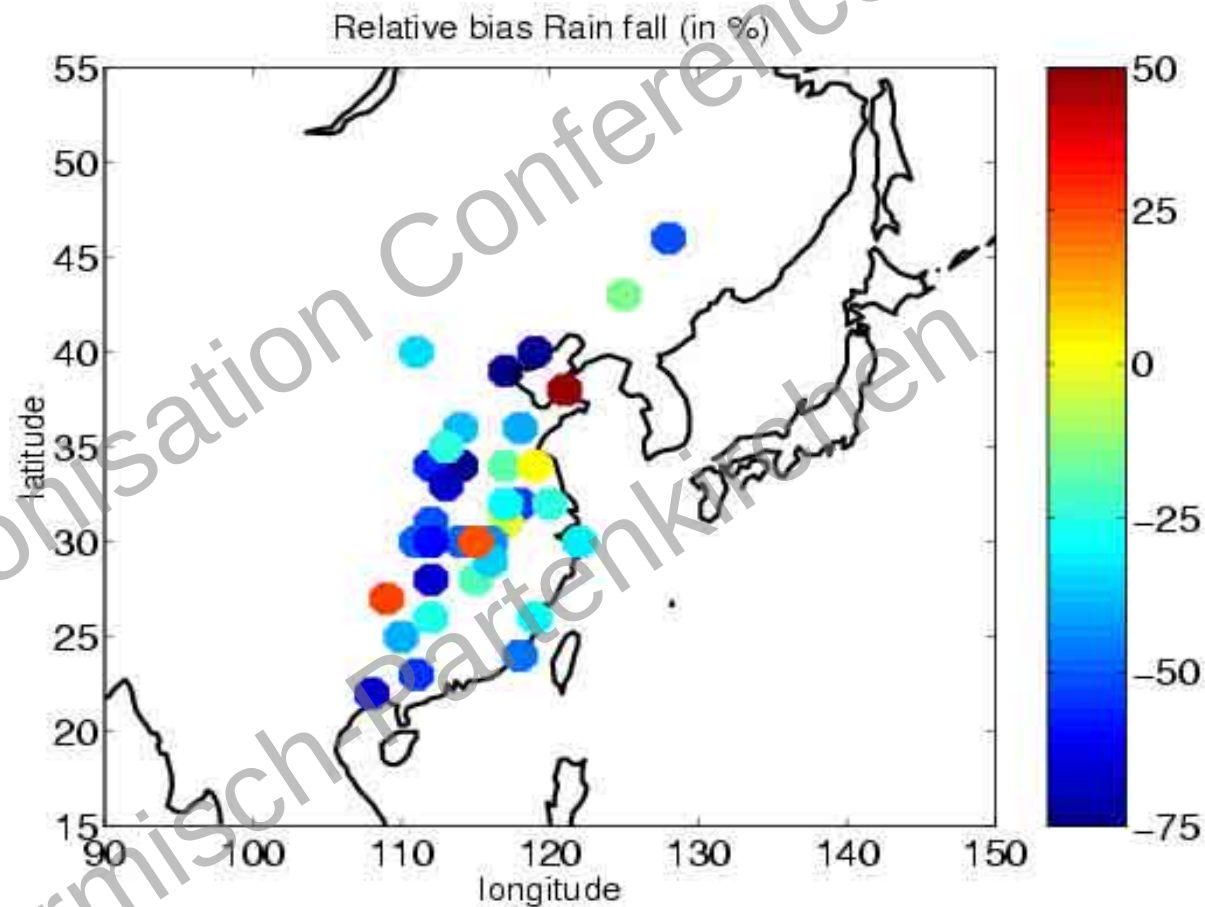


➔ **Under-estimation of the SO4 in the rain water**

➔ **A part due to the rainfall data**

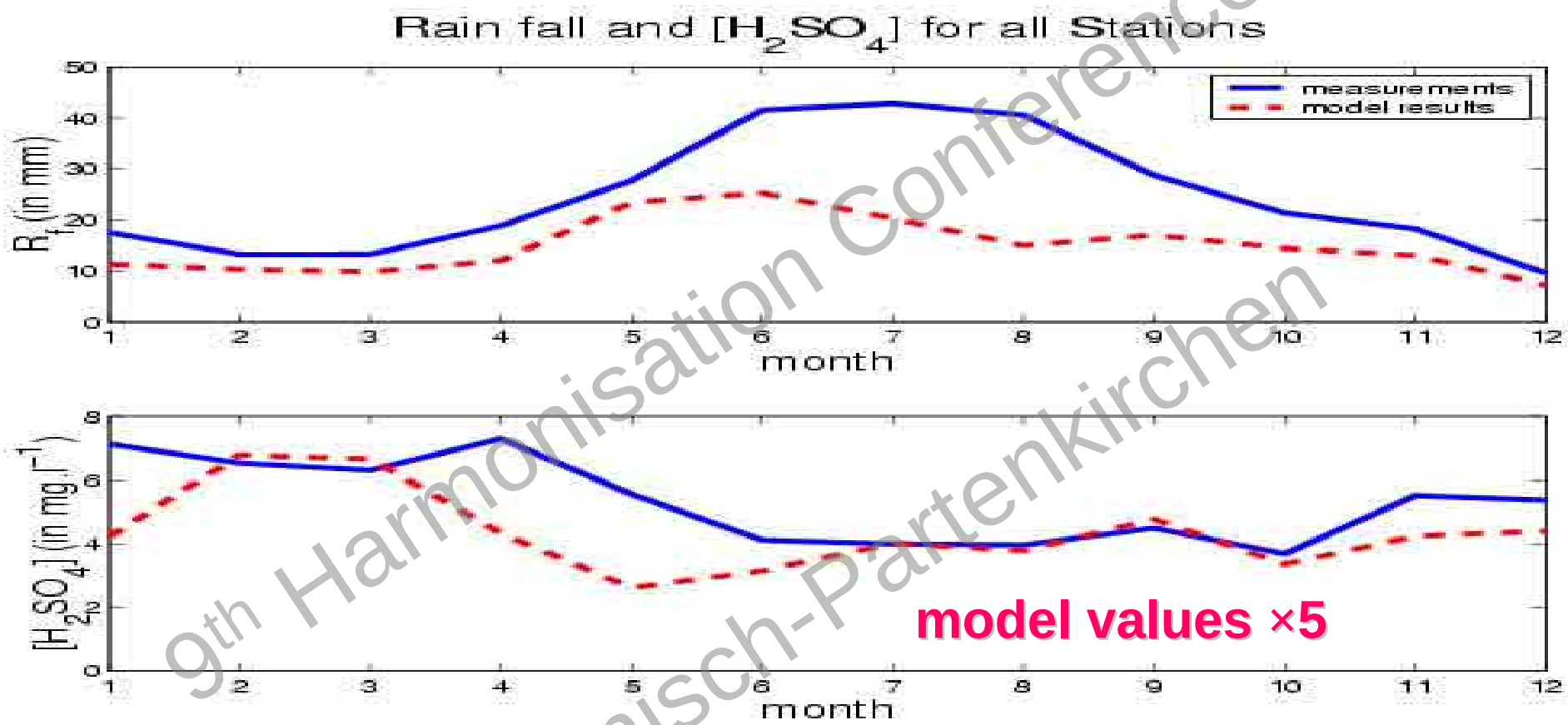
Rainfall bias

- **1200 « episodes » over 54 sites.**



➔ **High under-estimation of rainfall when using ECMWF coarse data**

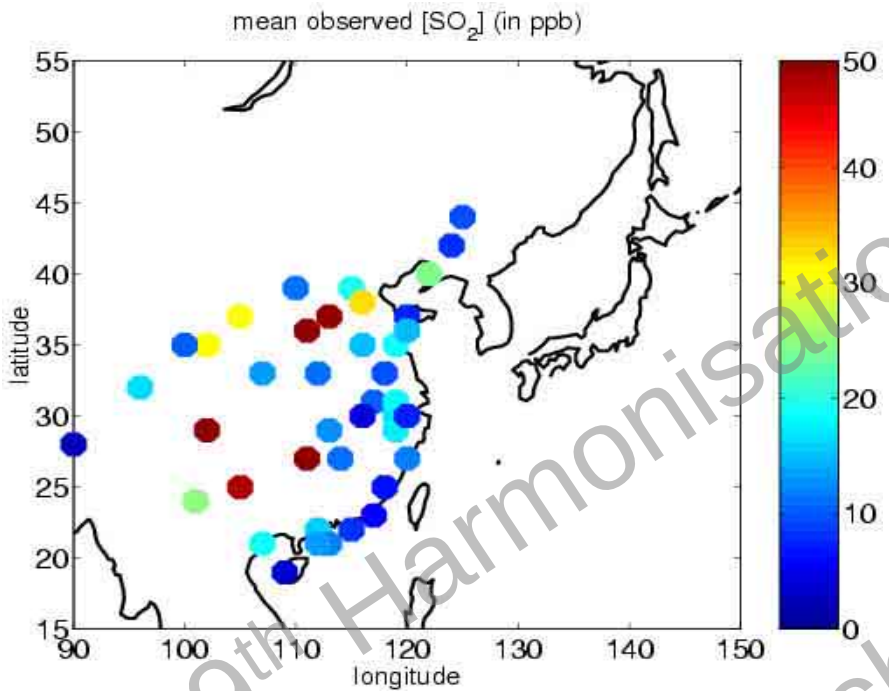
Season cycle

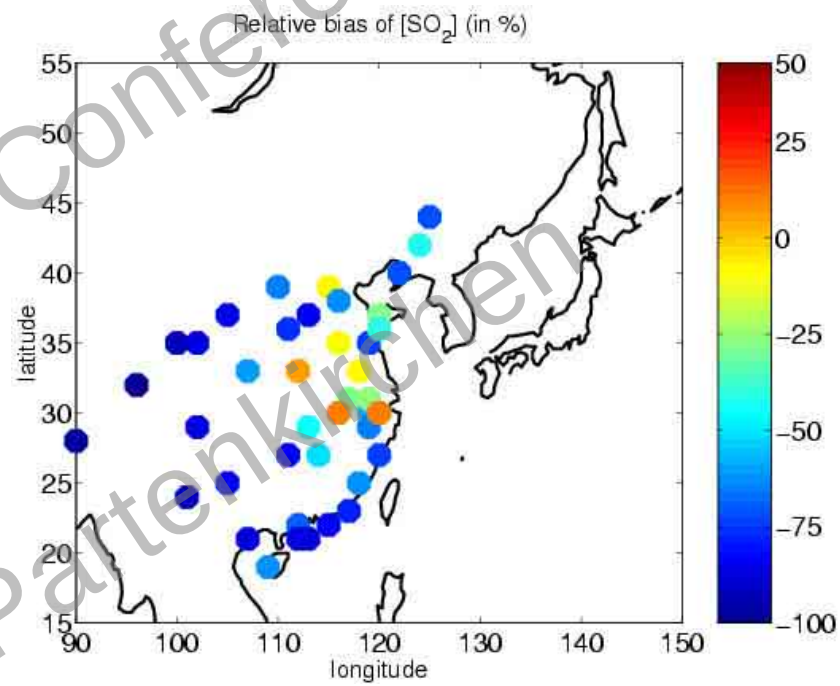


➔ **Summer : Rain ↗, SO4 concentrations ↘**

➔ **Winter : Rain ↘, SO4 concentration ↗**

[SO2] air concentration

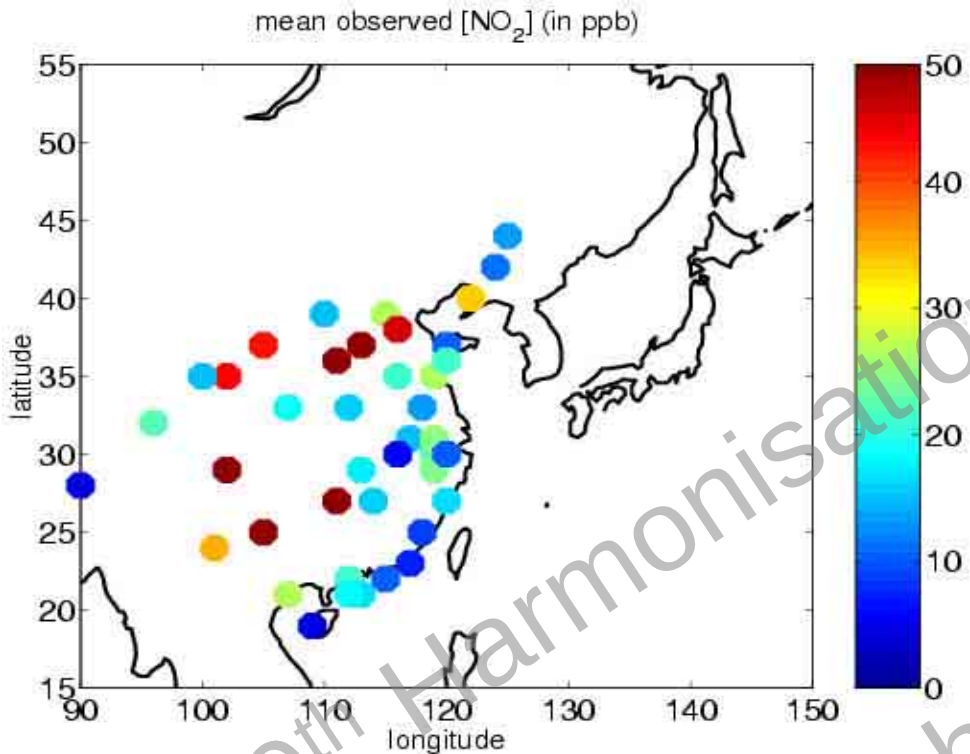


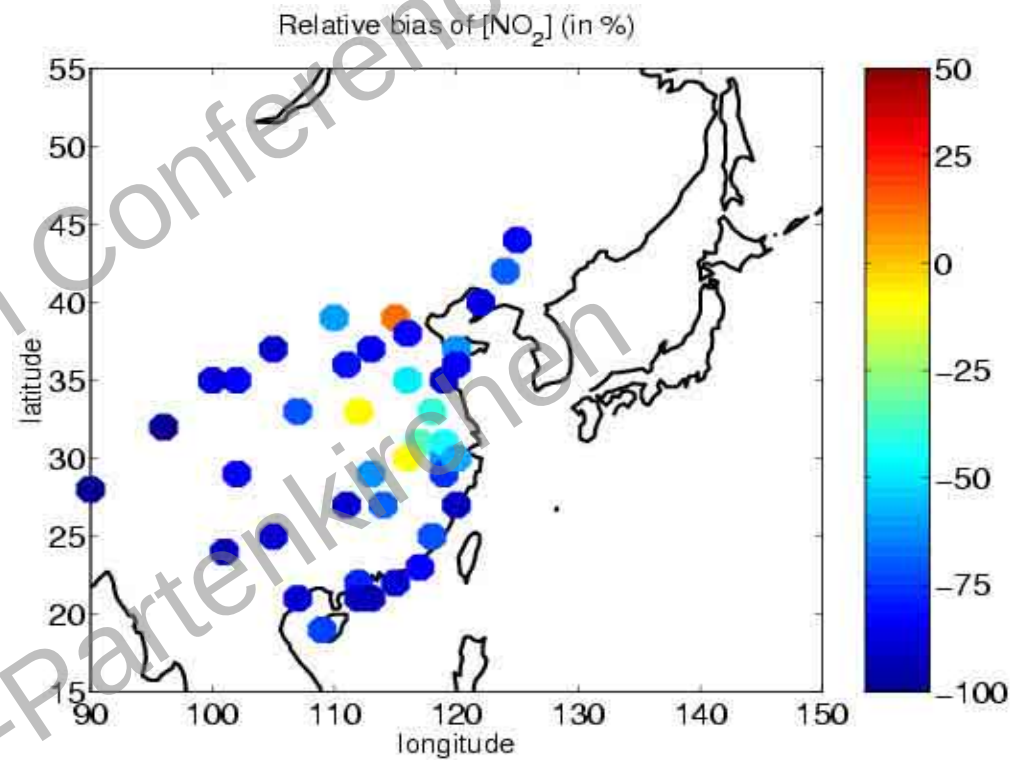


- ➔ **Question of Urban or background measurements (Continental scale)**
- ➔ **Spatial distribution OK**

- **Mean concentration from june 2000 to december 2000**

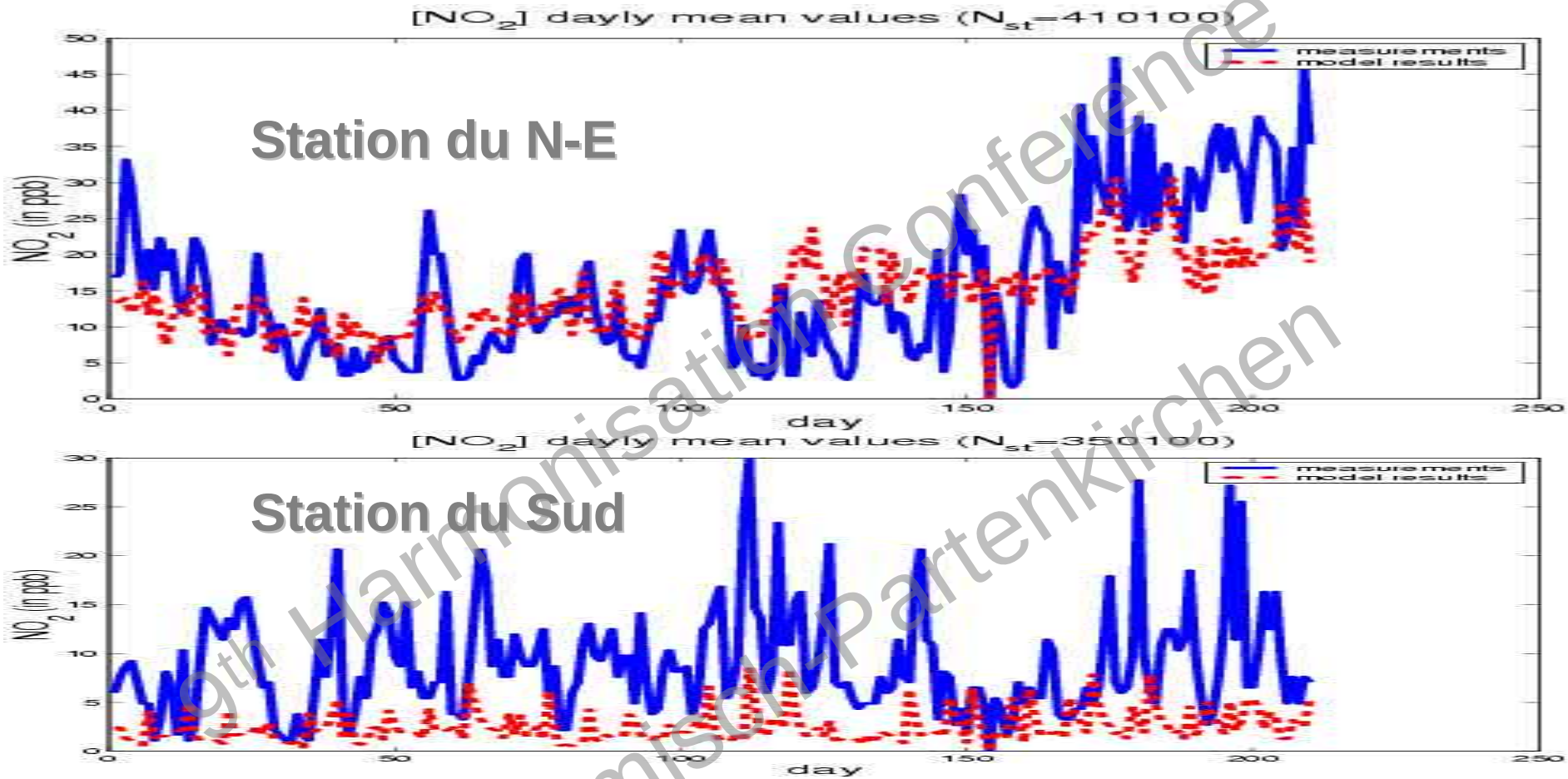
[NO_2] air concentration





➔ **Question of Urban or background measurements (Continental scale) (traffic ?)**

Time Series Examples

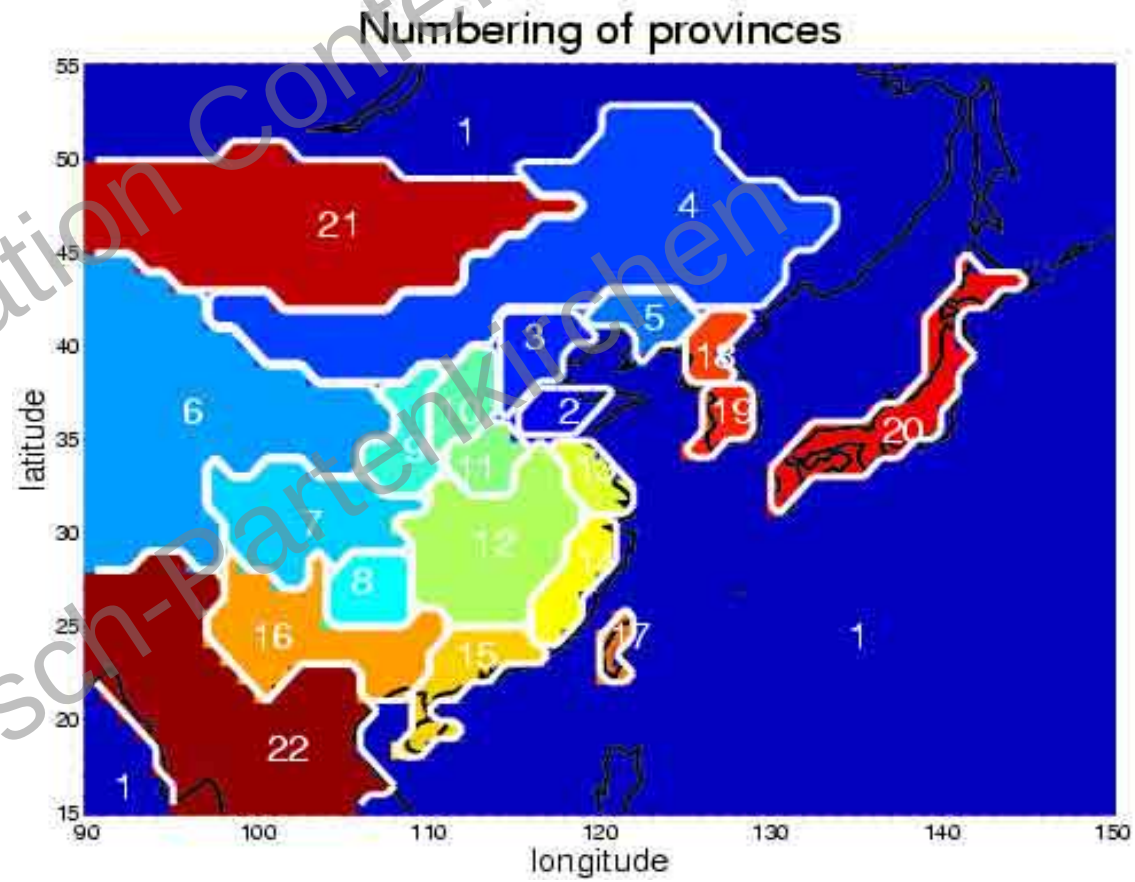


- **NE: Bias OK season cycle to be improved (model resolution ?)**
- **Au S et S-O : High Bias (emission ?)**

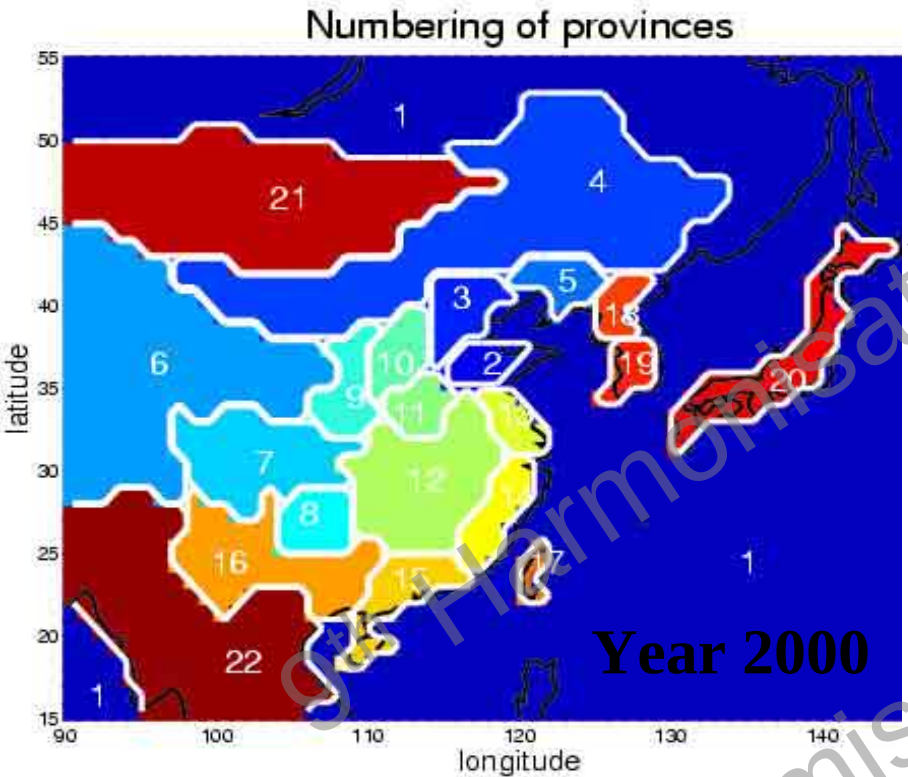
Evaluation pollutant fluxes exchange between geographical zones

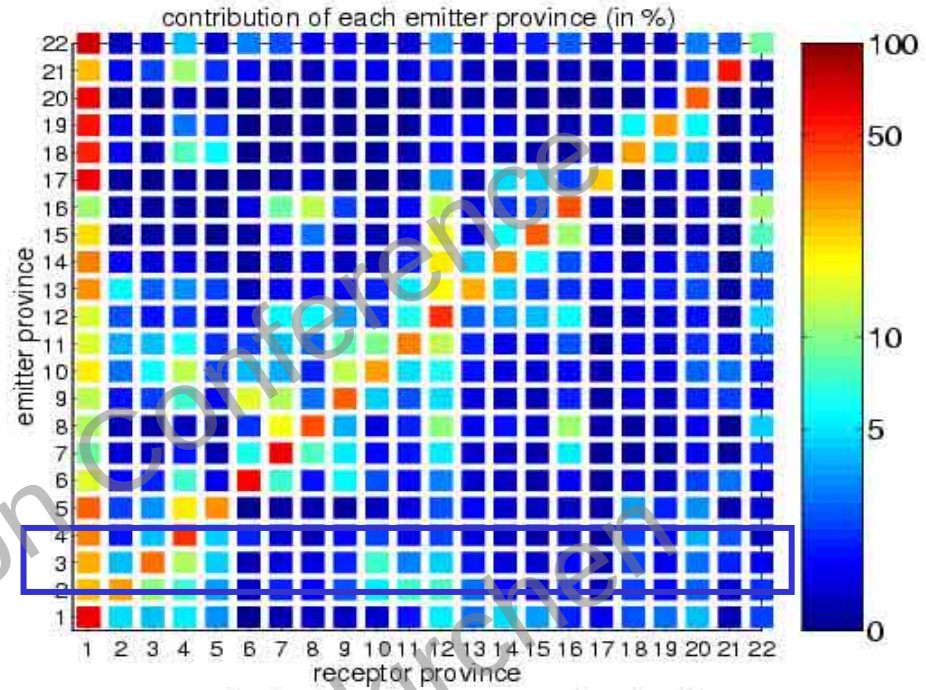
Area definition

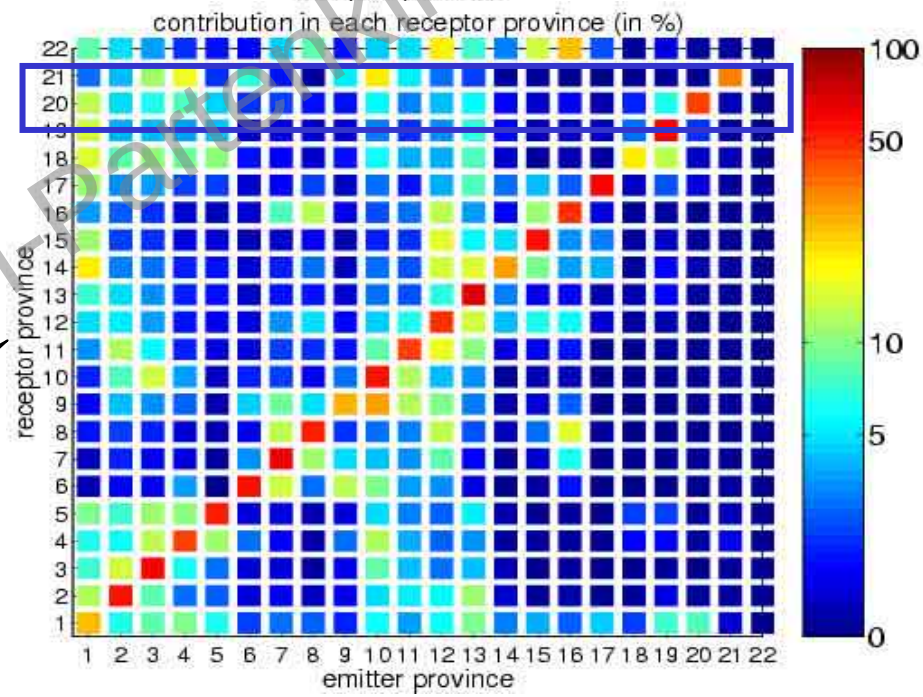
	Nom des province
1	Le reste
2	Shandong
3	Hebei, Beijing,Tianjin
4	Jilin, Neimenggu, Heilongliang
5	Lianing
6	Xinjinag, Quinghai,Xizang, Gansu, Ningxiahu
7	Sichuan, Choncquing
8	Guizhou
9	Shaanxi
10	Shanxi
11	Henan
12	Hubei, Anhui, Hunan, Jiangxi
13	Shangai, Jiangsu
14	Zheijang, Fujian
15	Guanghing, Hainan
16	Yunnan, Gangxi
17	Taiwan
18	Corée du Nord
19	Corée du sud
20	Japon
21	Mongolie
22	Indochine



Where does the emitted SO_2 give acid rain ?







Where does the sulphur come from ?

Where does sulphur pollution come from?

22	7	4	3	1	1	1	3	7	1	3	4	19	6	2	13	23	1	0	0	0	0	0
21	2	3	10	15	1	6	1	0	4	19	4	2	1	0	0	0	0	0	0	0	32	0
20	12	4	5	7	3	1	1	1	1	4	2	3	4	1	0	1	0	1	5	43	0	0
19	12	3	3	3	3	0	0	0	0	2	1	2	6	1	0	0	0	2	60	1	0	0
18	14	7	9	8	10	1	1	0	1	5	3	3	7	0	0	0	0	19	12	0	0	0
17	10	2	3	1	1	0	1	1	0	2	1	3	7	2	3	2	60	0	1	0	0	0
16	2	2	1	0	0	0	6	12	1	1	2	12	2	1	10	46	0	0	0	0	0	0
15	10	1	1	0	0	0	0	1	0	1	1	14	4	4	57	2	2	0	0	0	0	0
14	19	2	2	1	1	0	1	2	0	2	1	13	14	27	9	2	3	0	1	0	0	0
13	6	4	2	1	1	0	1	1	0	2	1	6	71	2	1	1	0	0	1	0	0	0
12	4	4	2	1	1	0	2	4	1	3	5	46	13	3	5	5	0	0	0	0	0	0
11	2	11	5	1	0	0	1	1	1	8	43	15	9	0	1	1	0	0	0	0	0	0
10	1	7	13	2	0	1	1	1	2	55	11	3	2	0	0	0	0	0	0	0	0	0
9	1	3	2	2	0	3	8	4	26	27	11	8	2	0	0	2	0	0	0	0	0	0
8	1	1	1	0	0	1	12	49	1	2	2	12	1	0	2	14	0	0	0	0	0	0
7	0	1	1	0	0	2	63	11	4	3	2	7	1	0	0	5	0	0	0	0	0	0
6	0	1	1	3	0	54	13	2	12	9	2	2	0	0	0	1	0	0	0	0	0	0
5	9	6	10	9	50	0	0	0	0	4	2	2	4	0	0	0	0	1	1	0	0	0
4	5	5	12	44	10	2	1	0	2	11	3	2	2	0	0	0	0	1	1	0	1	0
3	6	13	58	5	2	0	0	0	1	7	3	2	3	0	0	0	0	0	0	0	0	0
2	11	53	7	2	2	0	1	0	0	4	4	4	10	0	0	0	0	0	0	0	0	0
1	24	5	7	8	5	1	2	2	1	5	2	5	9	2	3	2	3	1	6	7	0	0
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22

Next steps ?

Next steps ?

- Focus on one or two target area
  - Improve resolution (10 to 5 km)
  - Nested in the CHIMERE-CHINE 2.0
  - Using a more precise emission inventory
- Desert Sand dispersion
  - Emission evaluation
  - Test of operational Forecasting
- PM 10 new developement