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# Modelling long-range transport and chemical transformation of pollutants in the southern Africa region

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# Outline

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  - *Surface roughness*
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# Long Range Transport?

- "long range (or regional) transport (>100km); e.g. the area in which large-scale meteorological effects, deposition and transformation rates play key roles" *Zannetti, 1990.*
- Atmospheric pollutants have variable residence times in the atmosphere.
- Transport over long distances.
- Typical distances where the dynamics of Gaussian plume models fail.
- Puff model dynamics addresses this need.



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# LED Model

- Lagrangian-Eulerian Diffusion (LED) Model.
- Puff based model utilizing in a complementary way the positive features of the Lagrangian and Eulerian description of hydrodynamic flows.
- *Lagrangian* method – Studying the properties variation of a fixed fluid volume during its motion. Any volume of polluted air is identified by the trajectory of its center of mass.
- The diffusion process of the polluted air are solved through differential equations in *Eulerian* coordinates, with the origin the center of mass.



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# Planetary Boundary Layer

- Unique feature of the LED is the solving of the ABL dynamics.
- Normal long range models utilize free atmospheric parameters (geostrophic wind velocity) available from meso scale meteorological models.
- Serious simplification since the changes in wind velocity and atmos. stability in the ABL dramatically influences the transport and diffusion processes.
- Frequent inversion layers at the top of the ABL forces the diffusion and transport of pollutants to take place in the lower parts of the atmosphere.
- The value of the vertical exchange coefficient changes by order of magnitudes depending on the stability conditions in the ABL.



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# PBL

- The LED utilizes a two-layer parametric ABL model (*Yordanov et al*, 1983).
- ABL model is driven by:
  - *Geostrophic wind vector* ($\vec{v}_g$);
  - *Potential temperature at the top of the ABL* ($T_H$);
  - *Surface temperature* ($T_S$).
- From these variables local parameters being calculated:
  - *Coriolis parameter* – $f$;
  - *Roughness parameter* – $z_0$;
  - *Buoyancy parameter* - $\beta$;
  - *Rosby number* - $R_0$;
  - *External stratification parameter* – $S$.
- There parameters uniquely determine the turbulent regime in the horizontally homogeneous ABL.



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# Chemical Transformations

- Chemistry model based on a simplified version of the MCM (*Jenkin et al.*, 1997).
- Explicit mechanism not a lumped sum mechnaism.
- Complete mechanism for inorganic pollutants.
- Chemical reactions (kinetics) described as differential equations.
- Integration by FACSIMILE.
- FACSIMILE
  - *Fortran based, designed to solve stiff differential equations using a variable order Gear's method.*
  - *www.mcpa-software.com*



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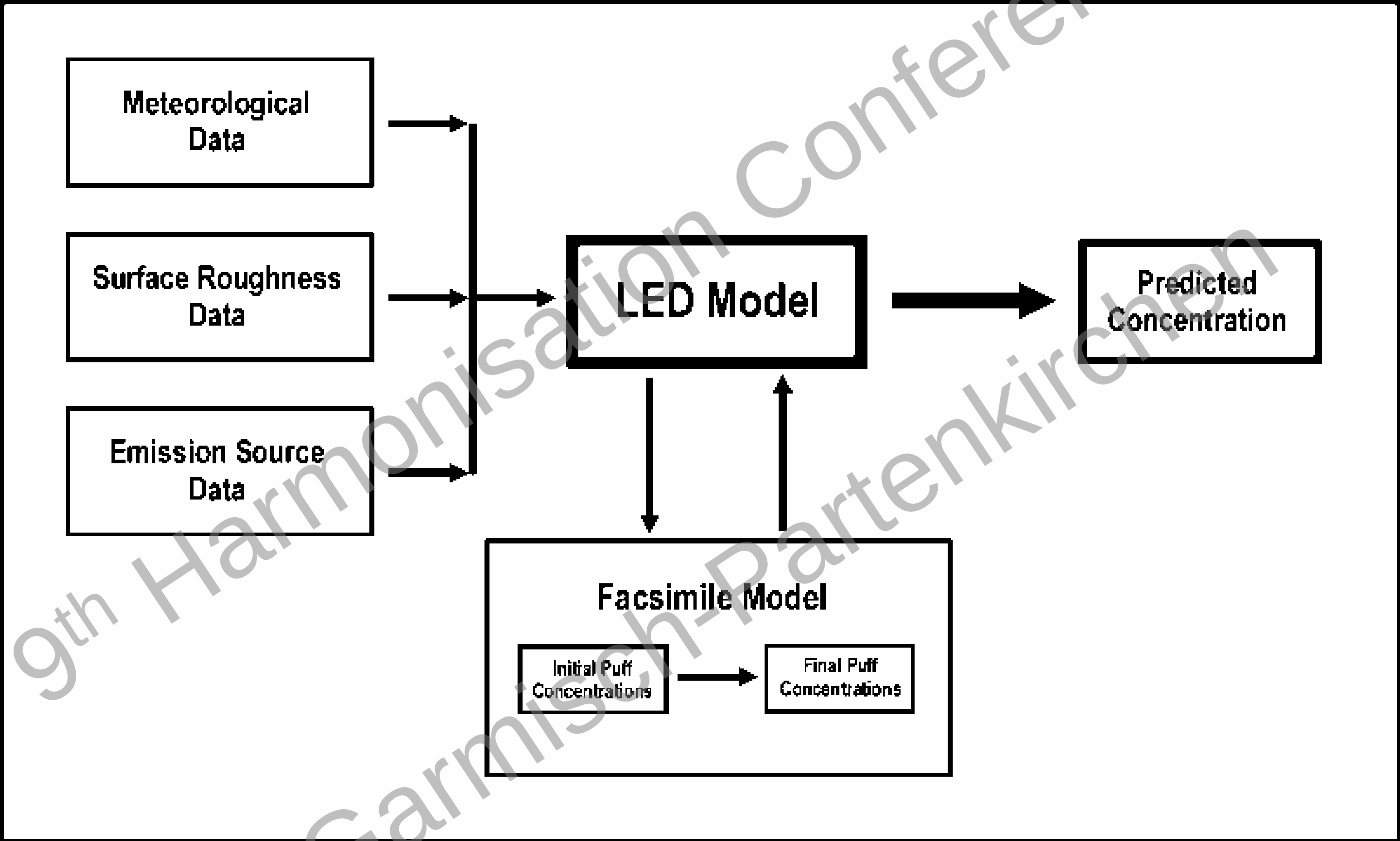
# Model Flow Diagram



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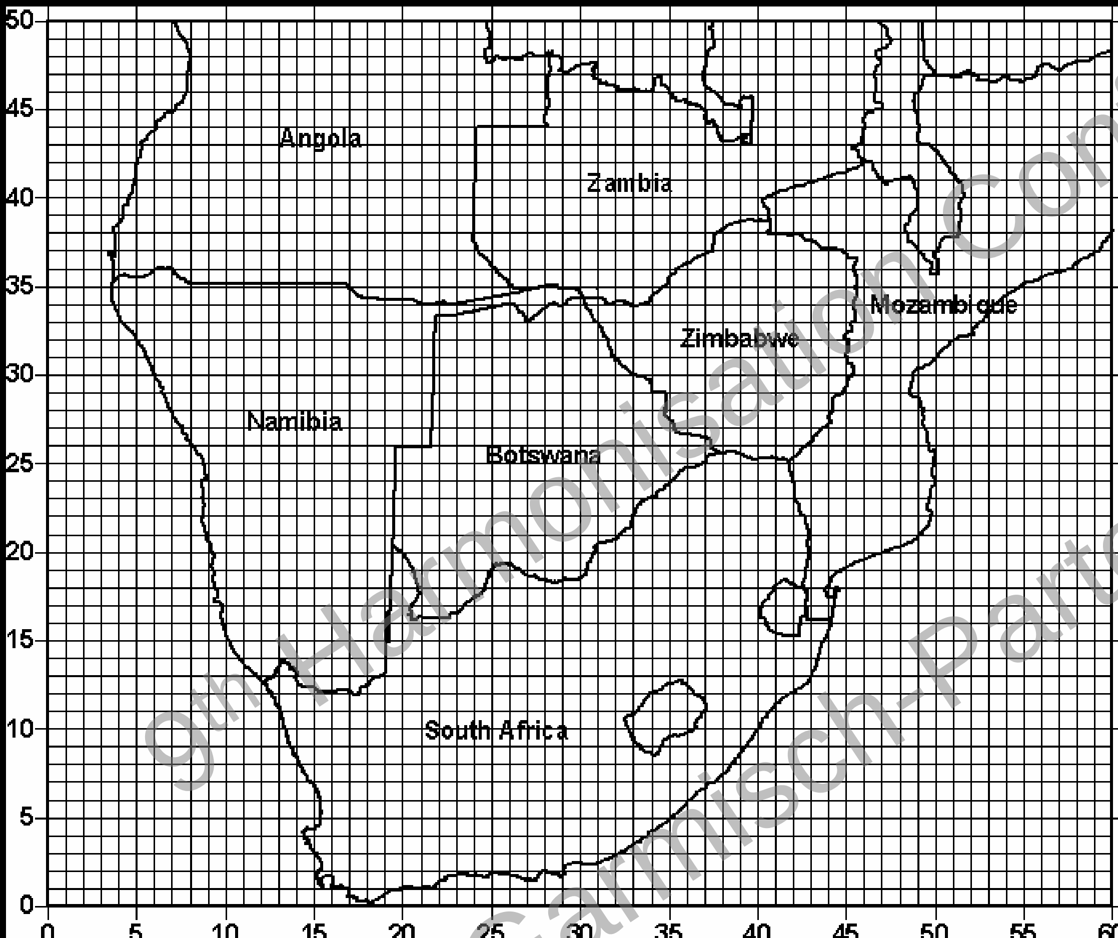
# Modelling Domain




- Southern African region.
- 10°E – 40°E; 10°S – 35°S.
- Grid 60 x 50 (0.5° Resolution).
- 50 x 50 km.



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# Meteorological Input

- Eta Model (South African Weather Service).
- The prognostic model in use is the NCEP regional eta- coordinate model with step-terrain representation.
- Integrated domain:
  - *Southern Africa and surrounding waters, transformed grid roughly contained in 52°S to 1°N, 28°W to 68°E.*
- Resolution:
  - *48km horizontally, with 38 eta levels in the vertical (top at 25hPa).*
- GRIB Eta Model Output (12-Hr):
  - *60 by 50 grid, 10°E – 40°E; 10°S – 35°S, half degree resolution.*
  - *700 hPa:  U, V and temperature components.*
  - *Ground level: Temperature component.*



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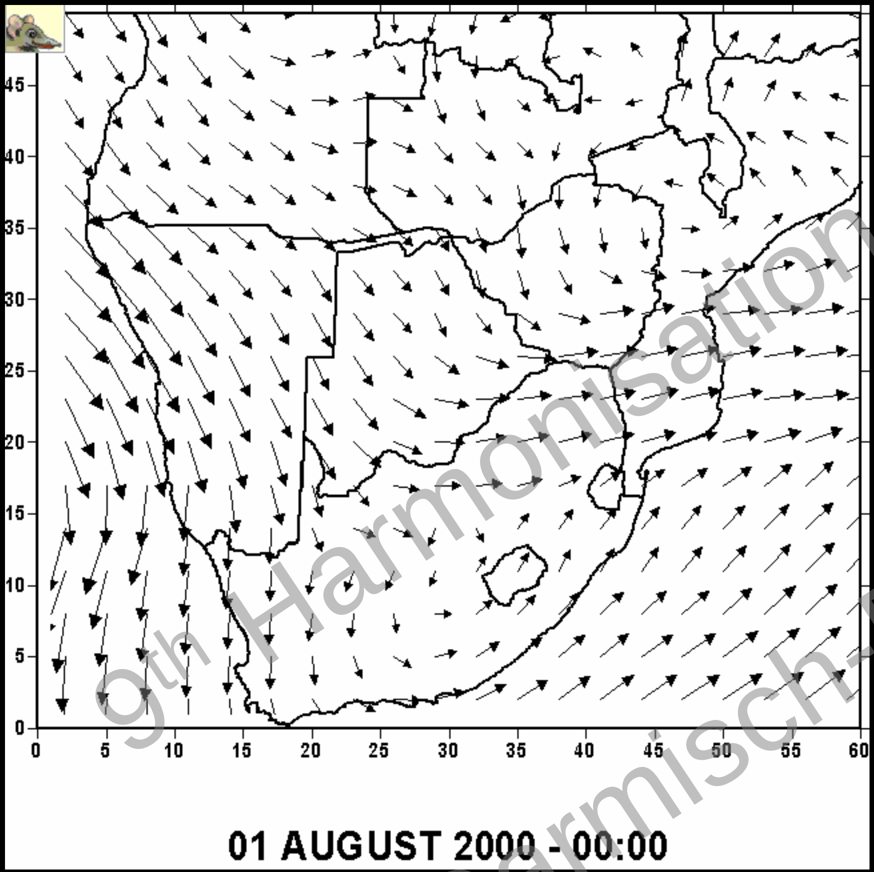
# Meteorological Input




- 60 by 50 grid, 0.5° resolution
- Geostrophic wind vectors (700hPa)



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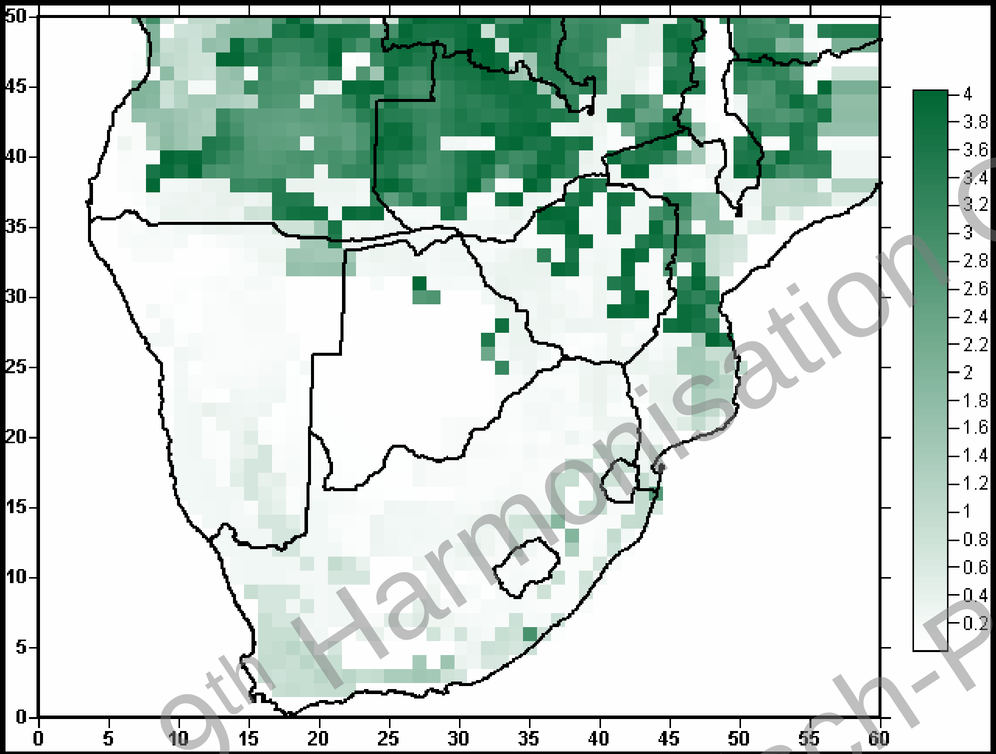
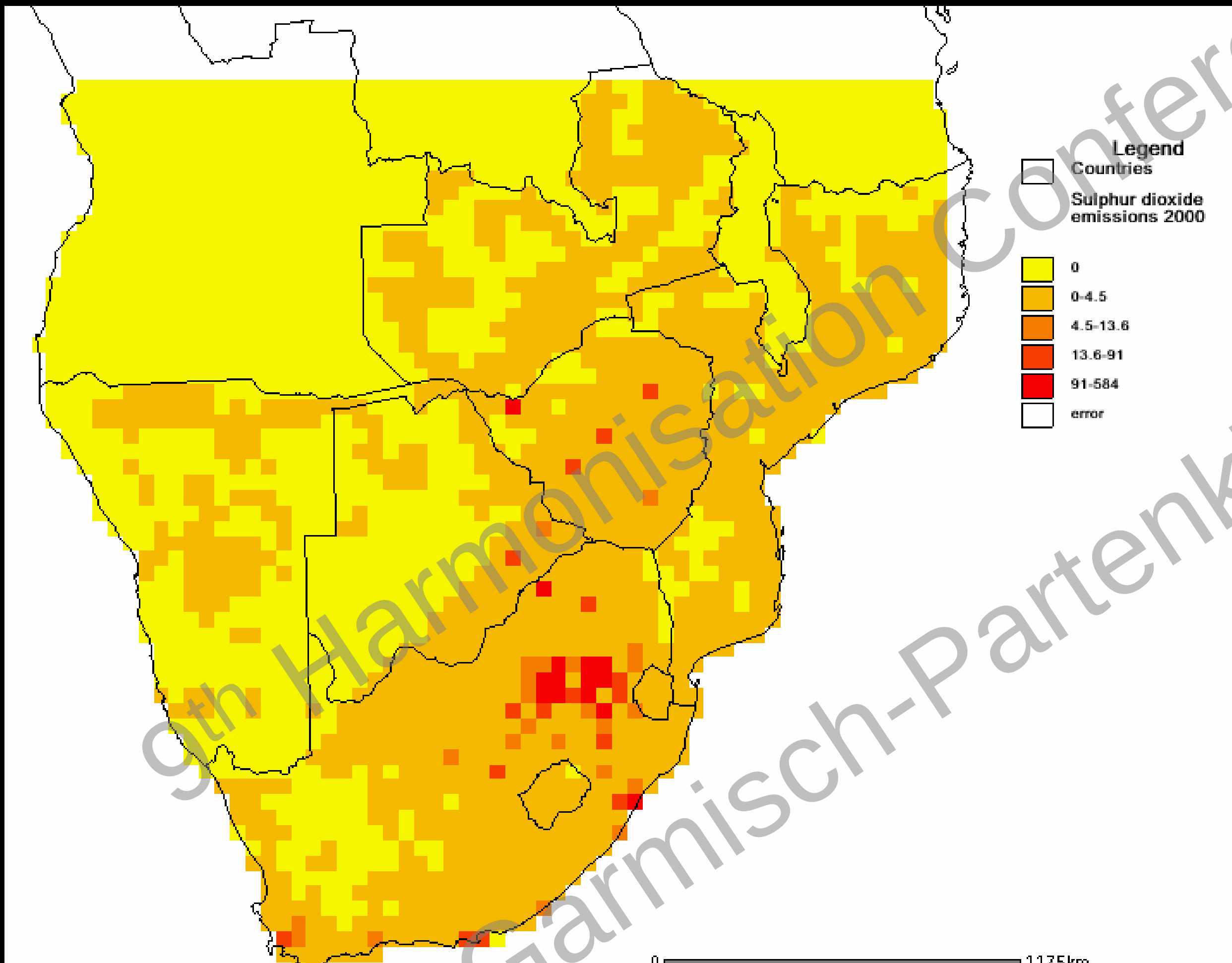
# Surface Roughness ($Z_0$)




- 60 by 50 grid, 0.5° resolution
- $Z_0$: August 2000 (m)
- Dr. L Ganzeveld
  - *Max Planck Institute, Mainz*

# Emission Sources




G Flemming & M Zunckel – CSIR South Africa

- SAFARI 2000
- Emissions:
  - $SO_2$
  - $NO_x$
  - $N_2O$
  - $CO$
  - $CO_2$
  - $CH_4$
  - $N\text{-}CH_4$
- 10°E – 40°E
  10°S – 35°S
  0.5° Resolution

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# Case Study

- Long-range transport of $SO_2$ over southern Africa
  - *60 x 50 grid (0.5° resolution).*
- Meteorological input from Eta model (12-Hr)
  - *August 2000 (1 month).*
- Emissions from SAFARI 2000 database
  - *Hourly emissions from 1363 sources;*
  - *Ellipsoid ($H_{Rad}$ – 28km, $H_{Vert}$ – 10m & $H_Z$ – 100m).*
- $Z_0$ data for August 2000.
- Complete inorganic chemical mechanism.
- No wet deposition / Only dry deposition.



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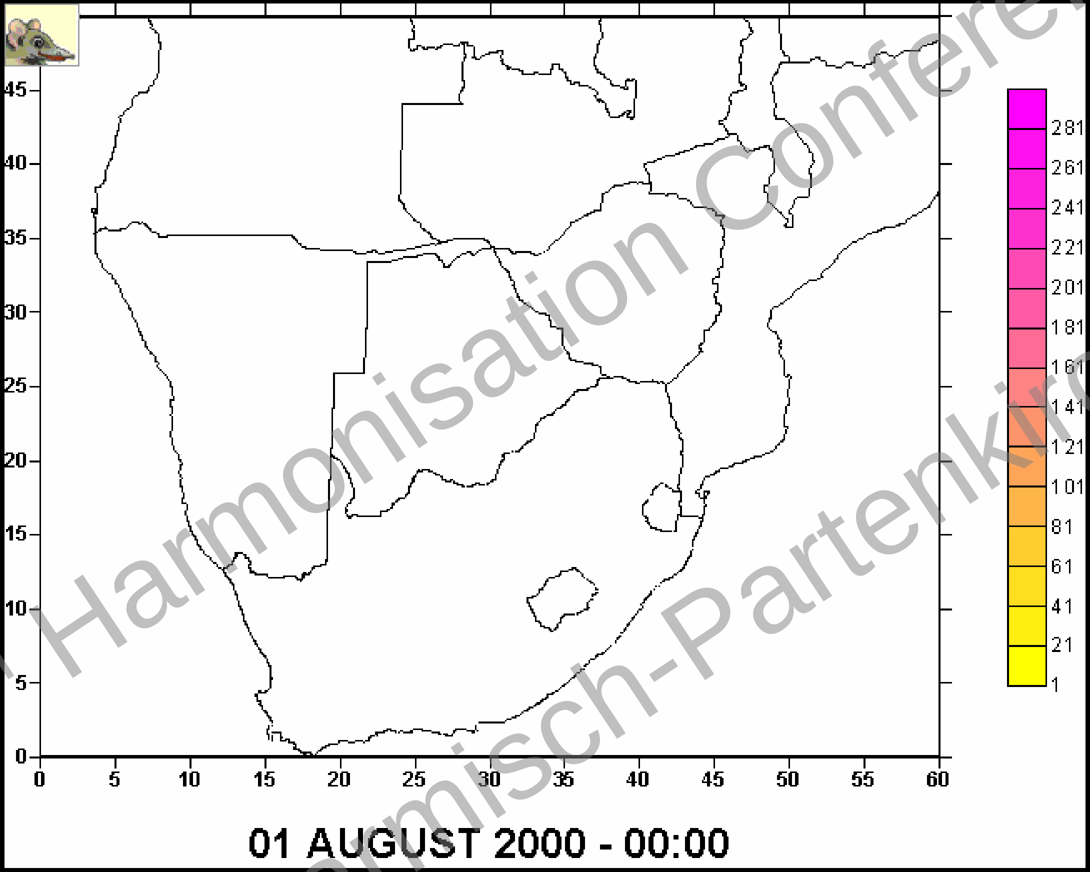
# Case Study - Results



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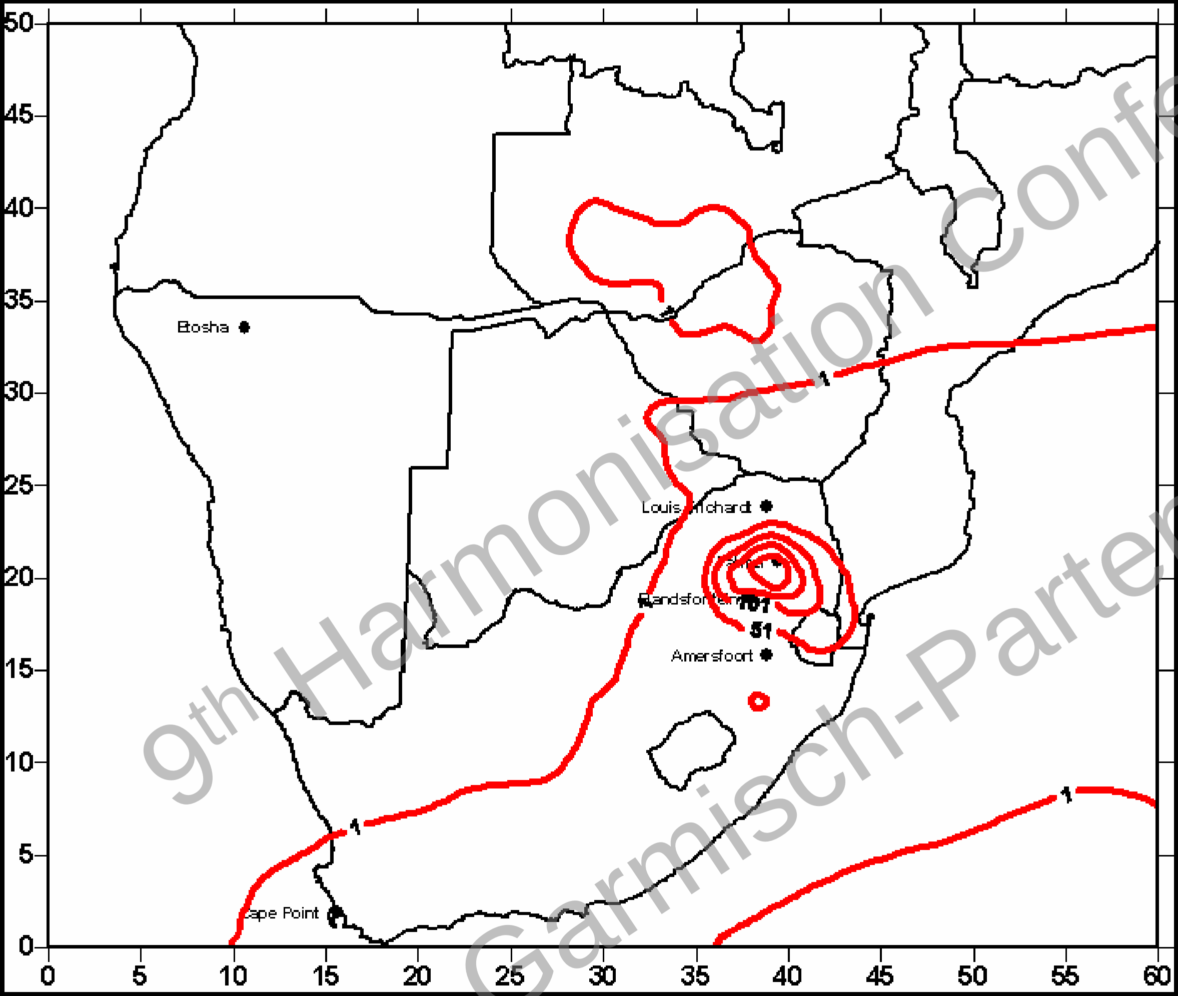
# Case Study - Results




- Mean $SO_2$ Concentration ($\mu g.m^{-3}$)



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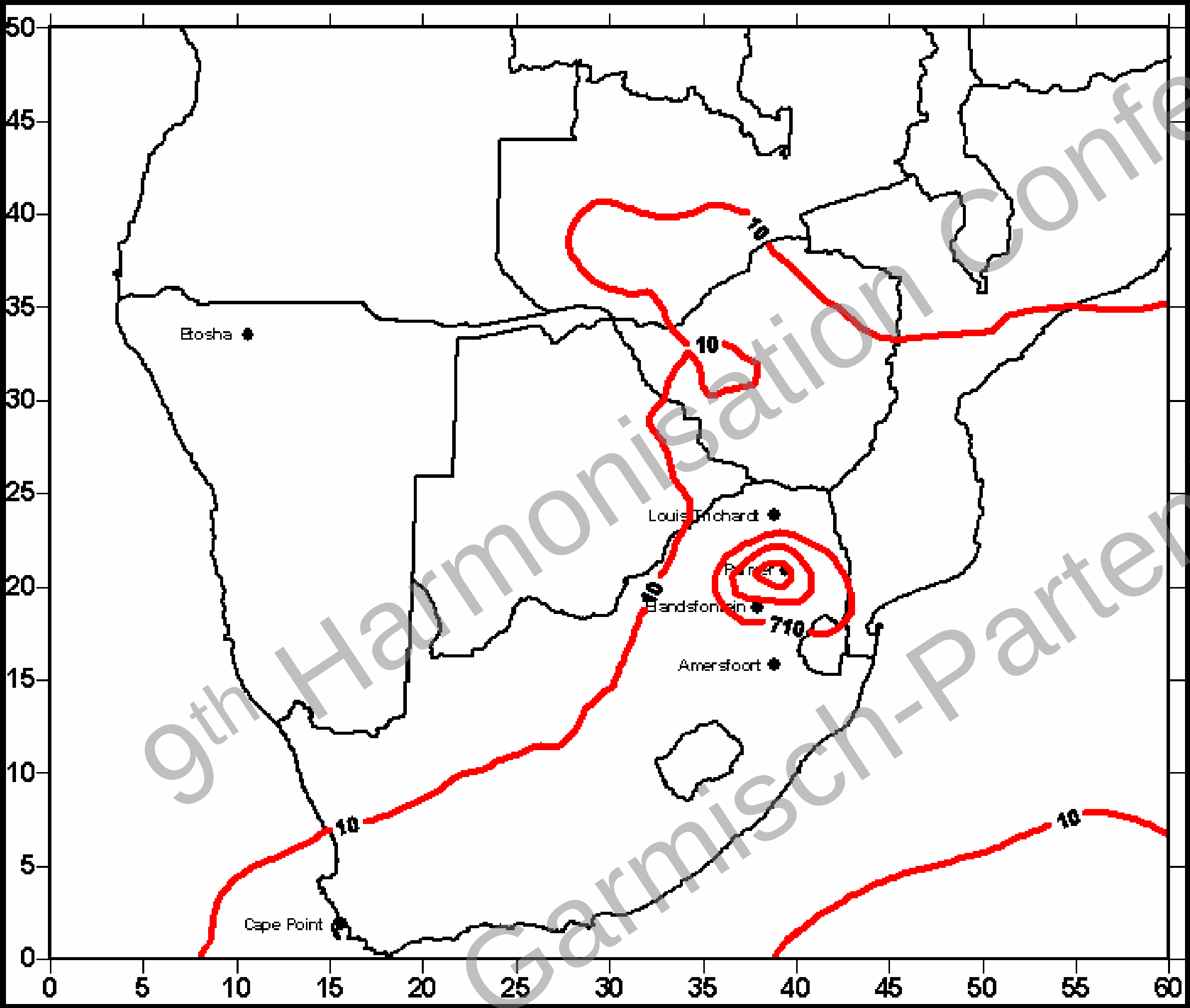
# Case Study - Results




- Mean $SO_2$ Dry Deposition ($\mu g.m^{-2}$)



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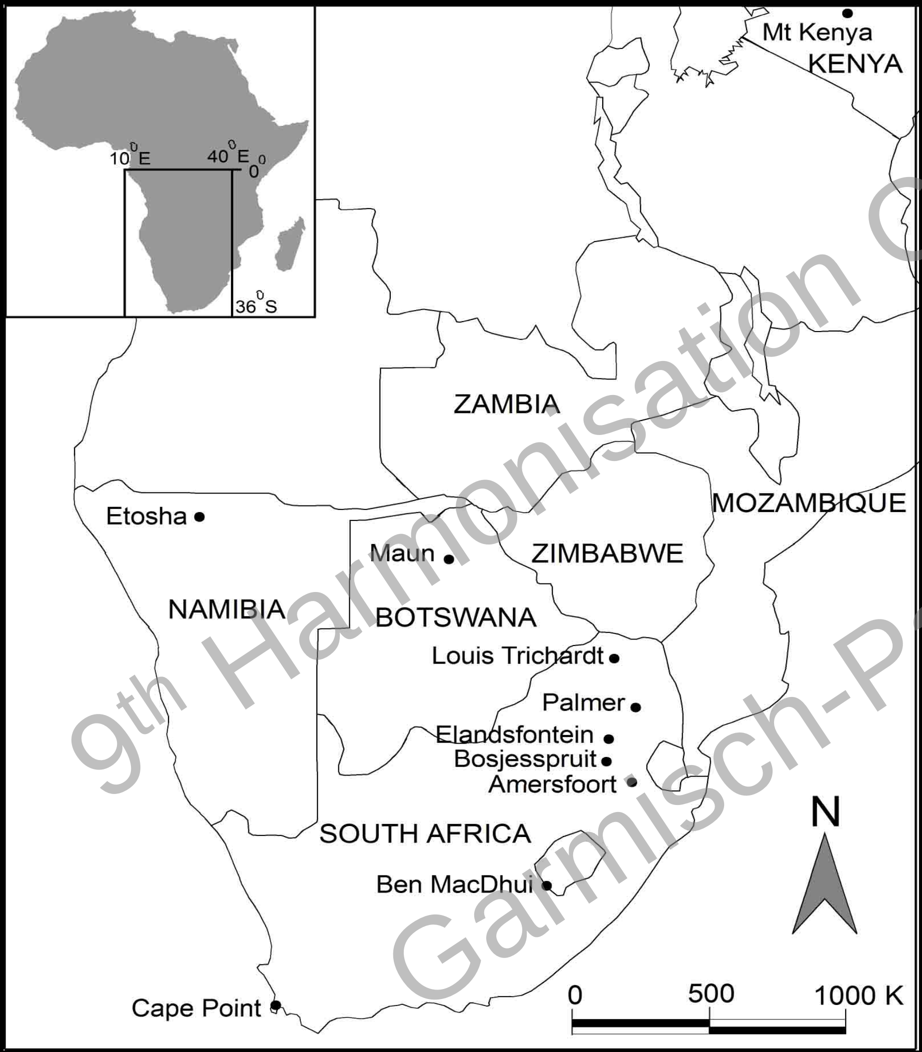
# Validation Study




- DEBITS Program
  - *IGAC Initiative*
- Stations:
  - *Cape Point*
  - *Etosha*
  - *Louis Trichardt*
  - *Palmer*
  - *Elandsfontein*
  - *Amersfoort*
- Species:
  - $SO_2$
  - $NO_2$
  - $NH_3$
  - $O_3$

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# Validation Study

- August 2000

| DEBITS Stations | DEBITS $SO_2$ Concentration ($\mu g.m^{-3}$) | Simulated Mean $SO_2$ Concentration ($\mu g.m^{-3}$) |
|---|---|---|
| Cape Point | 0.4 | 0.6 |
| Louis Trichardt | 0.6 | 5.7 |
| Palmer | 3.8 | 73.2 |
| Elandsfontein | 10.6 | 13.0 |
| Amersfoort | 2.6 | 4.6 |



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# Validation Study

| DEBITS Stations | $SO_2$ Dry Deposition ($mg.m^{-2}$)* | Simulated Mean $SO_2$ Dry Deposition ($mg.m^{-2}$) |
|---|---|---|
| Louis Trichardt | 2.8 | 4.1 |
| Palmer | 2.7 | 35.5 |
| Elandsfontein | 5.7 | 6.8 |
| Amersfoort | 3.0 | 3.2 |

* *Mphepya et al.*, 2002

# Conclusions

- The model can successfully simulate long range transport of air pollutants over southern Africa.
- The structure of the model allows for incorporation of a complete explicit chemical mechanism.
- The comparison with the available experimental data is quite satisfactory.

# Next Steps

- Wet deposition properties.
- Country to country deposition matrix
- Incorporate organic chemistry model:
  - *Biomass burning events;*
  - *Tropospheric ozone formation over southern Africa.*
- Study of pollution during prolonged gyre circulation.



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# Acknowledgements

**The research work has been supported by the National Research Foundation (NRF), South Africa and the SIDA, Sweden Project 'Non-local turbulent transport in weather prediction and air pollution modelling' SRP-2000-036 (South Africa-Swedish Research Partnership Programme 2000).**

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