# MODELLING THE MACROSCALE TRANSPORT OF SULPHUR DIOXIDE EMISSIONS FROM THE HIGHVELD REGION

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## INTRODUCTION

Anthropogenic sulphate aerosols have been implicated as an important factor in the global energy balance[1]. Atmospheric aerosols influence the climate both directly, through the reflection and absorption of solar radiation, and indirectly through the modification of the optical properties and lifetimes of clouds. Aerosols in the atmosphere are believed to represent a negative radiation forcing mechanism. The increase in anthropogenic aerosol emissions may thus particularly offset the increase in radiative forcing, and concomitant global warming due to elevated concentrations in greenhouse gasses.

An understanding of the impact of anthropogenic sulphate aerosols necessitates three fields of study: first, the quantification of sulphur emissions through the establishment of a source inventory; second, the characterization of the source — receptor relationship through the modelling of transportation, transformation and removal processes; and finally the measurement of receptor concentrations.

South Africa has extensive coal reserves, most of which are found in the Highveld region. Several coal-fired power stations, as well as industrialized sites, including heavy steel industries, are located in this region. The burning of fossil fuels in these power stations is the major source of anthropogenic $SO_2$ in South Africa.

An emission inventory was compiled by the Department of Environmental Affairs and Tourism (DEAT) for the 1993 calendar year. It includes emissions from scheduled processes, including $SO_2$ emissions from power stations, listed in the Atmospheric Pollution Prevention Act 45 of 1965[2]. $SO_2$ emissions are averaged in tonnes per annum per 0.25° x 0.25° grid squares. Seven grid squares, containing all the elevated (> 200m above ground level) emission points, are identified as the highest $SO_2$ emission areas, accounting for 70% of total national $SO_2$ emissions.

The impact of $SO_2$ emissions from the Highveld region was addressed in a report by Tyson *et al.*[3]. This was the first report to assemble all related studies and information on the Highveld region environment, and to characterize the impact of emissions from the Highveld. A shortcoming of this report, however, is that it identified the Highveld region as a 'box' or closed area, approximately 200 x 200km, thus failing to consider the potential of pollutants being transported further afield.

Long range transport of $SO_2$ in Europe and America are well documented[4]. Recent local studies drew attention to the potential impact of $SO_2$ emissions, generated in Highveld region, on the Northern Province, parts of Kwazulu-Natal and the Free State[2]. The transport, dispersion and transformation of pollutants from source regions need to be considered on a broader scale (> 500km).

## PROBLEM STATEMENT

The aim of the pilot study presented in this paper is to characterize the transport of $SO_2$ emissions from the Highveld region under various synoptic conditions (a continental anticyclone and westerly wave) over Southern Africa using results from large scale trajectory modelling.

The pilot study forms part of a wider study which aims to ascertain the nature and extent of the transport, dispersion, transformation and removal of sulphate aerosols, generated in the Highveld region, over Southern Africa. The wider study has been divided into three distinct sections. All three sections have been researched separately, but have not yet been combined:

- * Trajectory modelling: determining three-dimensional transport of airborne material in the atmosphere.
- * Dispersion modelling: simulates dispersion of sulphate aerosols.
- * Chemical transformation modelling: simulates $SO_2$ to particulate sulphate ($SO_4^{2-}$) conversion.

All three sections result in complex, spatial data sets. A Geographic Information System (GIS) was chosen to store, collate and manipulate these data sets and to facilitate impact analysis. A GIS is a database system with specific capabilities for spatially referenced data, and operations for working with such data. The ReGIS software package was chosen for this research project. During the pilot study ReGIS was only used for visual representation of calculated trajectories. Therefore this article will not cover the specific capabilities of a GIS. Our pilot study addressed the first section i.e. determining three-dimensional transport of airborne material. The model selected was a kinematic forward trajectory model[5] which observed three dimensional wind field components to trace the movement of air parcels with time, up to ten days. The model uses European Center for Medium Range Weather Forecasts (ECMWF) data as input.

To reduce this problem to manageable proportions, simplifications were made.

- September 1992 was chosen for the pilot study. This month was chosen because the ECMWF data sets were available and because it was well studied during SAFARI'92, thus validation of results obtained will be possible.

- Only the major $SO_2$ sources were considered, grouped together in the seven grid squares referred to above (Figure 1). The source location was taken as the geometric center of the grid squares.
- The climatology over Southern Africa has been classified into five characteristic synoptic circulation patterns. Two of these patterns occurred during the chosen period, a continental anticyclone and westerly wave. Representative days were chosen for each of these patterns. For each pattern a case study was performed in which the transport of $SO_2$ was modelled. Two sets of 10-day forward trajectories were created from the seven source areas.

To calculate forward trajectories, certain parameters need to be established from the emission inventory. In the following section input parameters and the forward trajectory model will be discussed.

## DATA REQUIREMENTS AND METHODOLOGY

### Emissions inventory

The emissions inventory used in this study was compiled by the Department of Environmental Affairs and Tourism (DEAT) in 1994, and reflects emissions from scheduled processes, including elevated sources, listed in the Atmospheric Pollution Prevention Act 45 of 1965. This inventory applies for the 1993 calendar year, and is the most appropriate inventory to the chosen study period September 1992.

Total $SO_2$ emissions by scheduled industries are average in tonnes per annum per 0.25° x 0.25° area. The inventory further divides emission in three categories:

- Sources < 10m above ground level (AGL)
- Sources 10 - 200m AGL
- Sources > 200m AGL

The majority (70% of total) $SO_2$ emissions are associated with the third category, i.e. > 200m AGL[2]. The dominance of $SO_2$ emissions above 200m can be attributed to the relative scale of the biggest sources, that is those sources required to have stacks higher than 200m AGL (elevated sources). The seven grid squares, identified with the highest $SO_2$ emissions (Between 135,700 and 352,800 tonnes per annum) contain all the elevated (> 200m AGL emission points (Figure 1)[2].

The emission inventory was used to establish the following input parameters.

- The trajectory model requires latitude-longitude coordinates as starting points for the forward trajectories. These coordinates were obtained from the emission inventory, i.e. the center point of each of the 0.25° x 0.25° grid areas (Figure 1).
- Starting heights for the trajectories were determined, using a pressure-height equation. All trajectories start at a point > 200m above ground level. The pressure level varies according to the altitude. For the pilot study an arbitrary level of 800hPa was chosen for all trajectories. The height of the tall stacks varies between 250 and 300m.

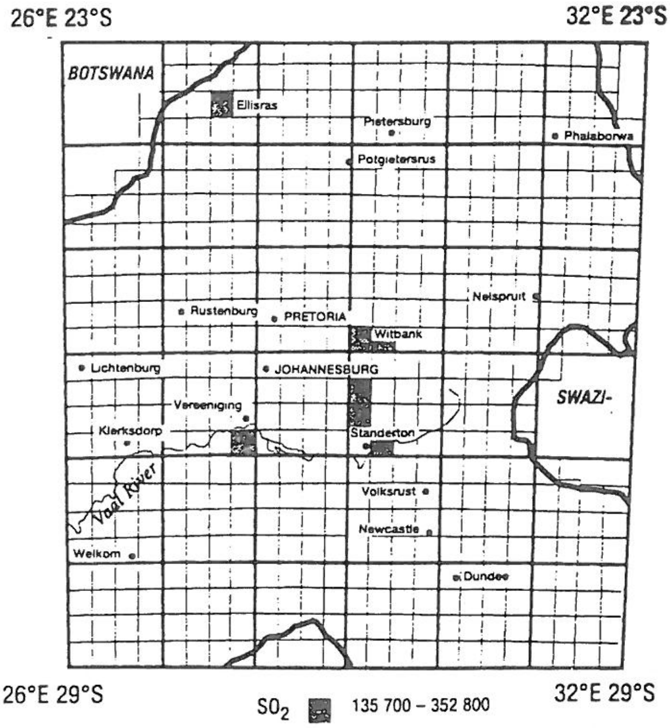

**Figure 1**: $SO_2$ tonnes per annum per 0.25° x 0.25° area[2].

### Trajectory analysis

Trajectory analysis is a useful tool for understanding the three-dimensional transport of airborne material in the atmosphere. Trajectories represent the paths of air-parcel movement, with time, resulting from changing synoptic circulation patterns.

Two variants of Lagrangian models are commonly used to construct three-dimensional trajectories, based on different assumption. Firstly, in the absence of vertical wind velocities, the isentropic assumption, that air parcels move along sloping constant-potential temperature surfaces, isentropic planes, is used to make direct estimates of vertical motions. Secondly, the kinematic approach uses the observed wind velocity components to trace the three-dimensional movement of air parcels[5].

The September 1992 data sets used were obtained from the European Center for Medium Range Weather Forecasts (ECMWF), by the Climatology Research Group, University of the Witwatersrand. The kinematic trajectory model utilizes twice daily (00:00 UT and 12:00 UT) ECMWF data for temperature, and u, v and w components for seven standard pressure surfaces on a 2.5° x 2.5° latitude-longitude grid. This data field is interpolated linearly from the seven initial pressure levels to ten equally spaced pressure levels from 1000hPa to 100hPa. Temporal interpolation is also performed tto obtain hourly temperature, and u, v and w wind components from the data sets[5].

September 1992 upper air meteorology data and synoptic charts were obtained from the Weather Bureau. Analyses of these data sets were done to identify days when each of the synoptic situations (a continental anticyclone and westerly wave) prevailed. The dates chosen for the case studies, i.e. starting dates for the trajectories, were:

- Continental anticyclone - 14/9/1992.
- Westerly wave - 21/9/1992.

Seven ten-day forward trajectories were modelled for each synoptic situation, each trajectory starting from a grid square identified from the emissions inventory. These sets of trajectories were all started at the same height, i.e. 800hPa, corresponding to average stack heights. These trajectory sets are assumed to simulate the movement of $SO_2$ from the Highveld region for the identifies synoptic situations.

## RESULTS

Forward trajectories calculated for each of the stated dates from the identified $SO_2$ source areas are displayed in figures 2 and 3. The trajectories represent atmospheric motion in terms of individual air parcel movement within air streams resulting form changing synoptic circulation patterns.

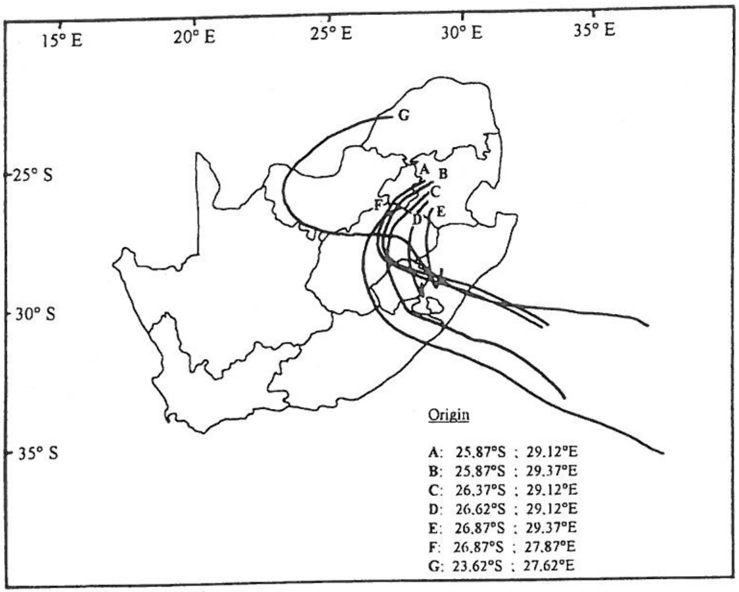

**Figure 2a**: Ten-day forward trajectories from seven identified $SO_2$ source areas, 14 September 1992, at 800hPa, during occurrence of a continental anticyclone.

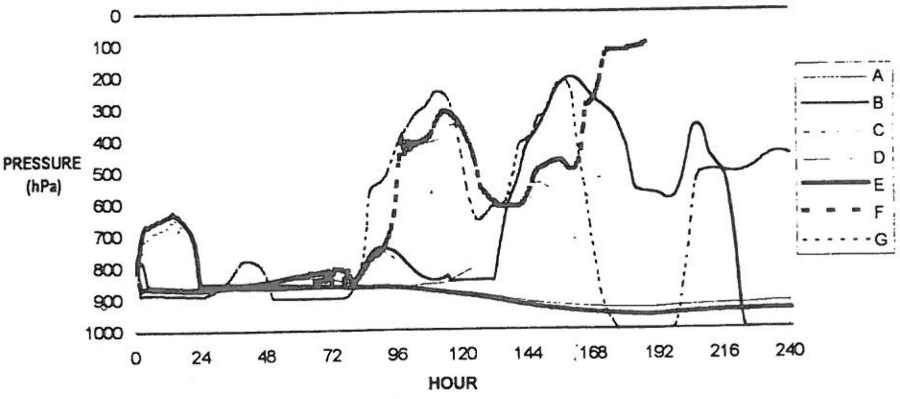

**Figure 2b**: Vertical movement of the seven forward trajecttories undertaken during occurrence of a continental anticyclone, in pressure units.

## DISCUSSION

A general anti-cyclonic circulation pattern can be distinguished when the continental anticyclone is present over the Highveld region (Figure 2a). Although there is a difference in endpoints and lengths of individual trajectories, a coherency exists between individual paths of each trajectory. The general trend is that the trajectories exit the continent after 4 days between the latitudes 30°S and 32°S.

Stable airflow occurs during the first three days with uplift being suppressed (Figure2b) during occurrence of continental anticyclone. Vertical mixing of air parcels occur from the fourth day when trajectories A, B, C and F exit the continent and are caught in a westerly wave.

When a westerly wave occurs, a coherent easterly movement (Figure 3a) is followed by all trajectories, exiting the continent after two days. All trajectories ascend for the first 24 hours (Figure 3b). Six trajectories ascend to 100hPa, where the kinematic forward trajectory model terminates calculations, by default.

## CONCLUSION

During the occurrence of the continental anticyclone over the Highveld region uplift is inhibited. Sulphur is at 800hPa, for three days available to be mixed downward by thermally or topographically induced turbulence. Under these conditions high ground level concentrations of $SO_2$ could occur, and dry deposition enhanced.

In contrast, during the occurrence of a cold front (westerly wave) over the Highveld region, the trajectories ascend rapidly, beyond the range of boundary layer mixing. Ground level concentrations and dry deposition are prohibited. Potential for conversion of $SO_2$ to $SO_4^{2-}$ is enhanced due to longer atmospheric residence time.

Following characterization of transport, the wider research project will focus on the dispersion and diffusion of $SO_2$ emissions from the Highveld region. The results from the trajectory analysis will serve as input into a puff

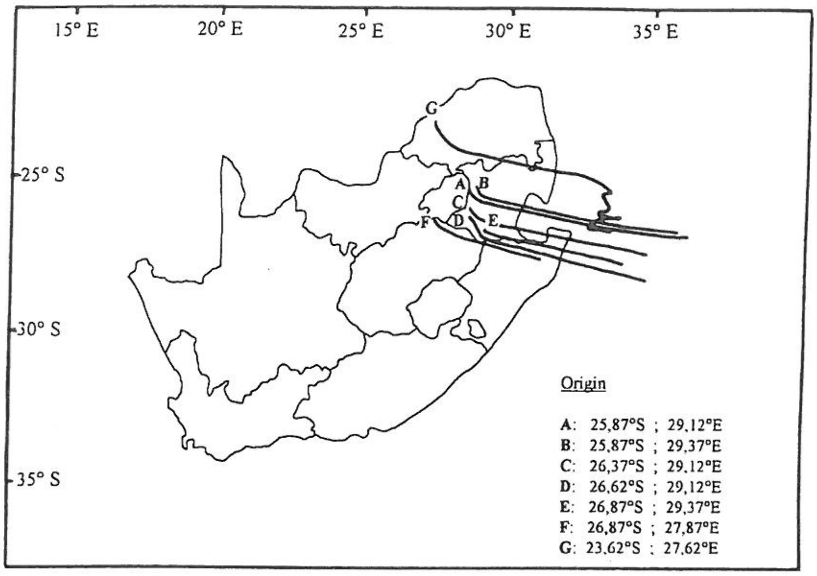

**Figure 3a**: Ten-day forward trajectories from seven identified $SO_2$ source areas, 21 September 1992, at 800hPa, during occurrence of a westerly wave (cold front).

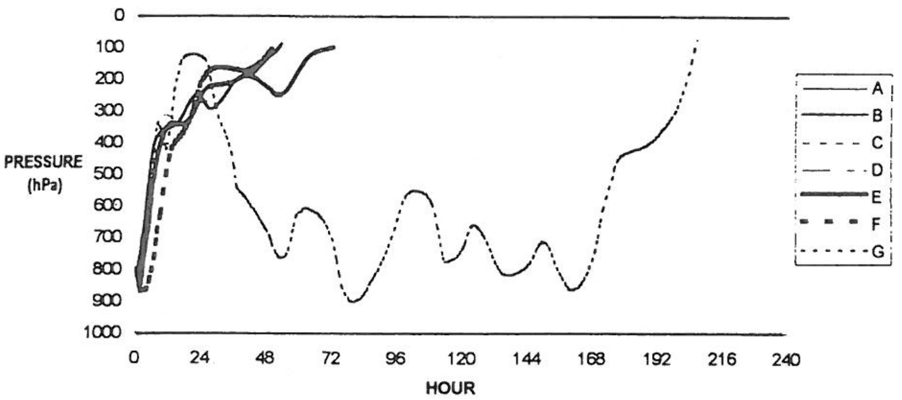

**Figure 3b**: Vertical movement of the seven forward trajectories undertaken during occurrence of a westerly wave, in pressure units.

dispersion model which will determine the dispersion and diffusion of $SO_2$ emissions along the identified transport paths. GIS will be used to give spatial analysis and predictions of ground level concentrations of $SO_2$.

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