Chapter 4

Direct comparison of airborne and ground based air quality data

Factors influencing the mixing in the troposphere, which in turn influences the agreement between airborne and surface monitored air quality data will be considered in this chapter. Direct comparison of airborne and ground based air quality data will be made.

Challenges of comparing airborne and surface monitored air quality data

The comparability of airborne air quality data to surface measurements is dependent on the extent of mixing of air in the troposphere. The mixing is in turn influenced by meteorological conditions, atmospheric lifetime of air pollutants, sources distribution and the height at which the pollutants are released into the troposphere (Annegarn *et al*., 1996a; Luke *et al*., 1998).

Influence of the diurnal evolution of the mixing layer on air dispersion

The diurnal evolution of the mixing layer plays an important part in the agreement between airborne and ground based measured air quality data (Luke *et al*., 1998). In the morning the surface emissions are trapped below a shallow mixing layer caused by the nocturnal near ground level inversion, and emissions from tall industrial stacks are prevented from mixing with the air below this inversion. The consequence of this nocturnal near ground level inversion is a decoupled lower and upper troposphere, which in turn lead to a vertical gradient or discontinuity in air pollutants concentration distribution. About mid-day the surface inversion is mixed out and the mixing layer is deep enough to allow air aloft to mix with surface air. This leads to a deep mixing layer with air homogeneously mixed in vertical up to high altitudes (Turner, 1996; Luke *et al*., 1998), a favourable condition to compare the two data sets (Luke *et al*., 1998).

Table 4.1 shows the data that were collected in the morning over Secunda during the Highveld autumn campaign. The data were collected on 18/03/2005 approximately at 167 magl, 333 magl and 667 magl flight levels, from 10:35:00 to 12:37:45 (SAST). Data from industrial plume penetration incidences are included in this data set. On 18/03/2005 Secunda was under the influence of surface trough as is shown on Figure 3.1(c). In the morning the surface was capped by a nocturnal ground level inversion at 92 magl (Figure 3.2(a)), which was mixed out in the afternoon resulting a deep mixing layer which was capped by an inversion at 2775 magl (Figure 3.2(b)).

The uneven vertical distribution of air pollutants levels in the morning is clearly evident in Table 4.1. The air pollutants were not well mixed within the column that was monitored. The SO_2 and NO_X average concentrations were relatively lower at 167 magl, and relatively higher at 333 magl and 667 magl and their maximum values indicate penetration of industrial plumes from the Secunda tall industrial stacks (Freiman and Picketh, 2002). O_3 was only slightly higher at 167 magl than at the two higher flight levels because of destruction by NO (Kley *et al*., 1994; Poulida *et al*., 1994; Hobbs *et al*., 2003, Taubman *et al*., 2004) from tall industrial stacks. This uneven concentration distribution in the vertical can lead to disagreements between airborne and surface air quality measurements.

Table 4.1: Air pollutants levels over Secunda at different heights in the morning

Pollutant	Min Conc (ppb)	Max Conc (ppb)	Avg Conc (ppb)	StdDev %	Height (magl)
O_3	16.37	86.201	34.506	39.196	167
NO_X	0	8.262	2.518	72.681	167
SO_2	2.605	65.775	19.352	77.65	167
O_3	8.679	77.037	31.409	49.284	333
NO_X	0.186	24.443	10.188	54.871	333
SO_2	3.895	157.724	63.733	64.232	333
O_3	13.151	64.588	32.415	32.083	667
NO_X	0	16.811	8.644	49.179	667
SO_2	3.555	131.753	55.449	64.87	667

Table 4.2 shows the data that were collected in the afternoon over the Vaal Triangle during the Highveld autumn campaign. The data were collected on 17/03/2005 approximately at 167 magl and 333 magl flight levels, from 15:17:00 to 16:53:30 (SAST). Data from industrial plume penetration incidences are included in this data set. Like in the Secunda case study the Vaal Triangle was also under the influence of the surface trough (Figure 3.1(b)). In the morning the surface was also capped by a nocturnal inversion at 276 magl (figure 3.2(a)), which was mixed out in the afternoon resulting a deep unstable mixing layer (Figure 3.2(b)).

The uniform mixing in vertical in air pollutants levels in the afternoon can be clearly seen in Table 4.2. The air pollutants average concentrations were comparable at both monitoring flight levels, though their maximum values especially of SO_2 indicates penetration of industrial emissions from the Vaal Triangle tall industrial stacks. This homogeneity in the vertical in the afternoon favours the comparison of the airborne and surface air quality measurements (Luke *et al*., 1998).

Table 4.2: Air pollutants levels over the Vaal Triangle at different heights in the afternoon

Pollutant	Min Conc (ppb)	Max Conc (ppb)	Avg Conc (ppb)	StdDev %	Height (magl)
O_3	37.866	47.928	42.505	5.442	167
NO_X	0	0	0	0	167
SO_2	4.91	14.05	6.972	23.232	167
O_3	35.428	47.372	41.2113	5.916336	333
NO_X	0.006	3.96	1.994271	57.51993	333
SO_2	3.339	62.084	8.694359	106.3663	333

Spatial variation of air pollutants

Figures 4.1 to 4.3 show concentration frequency distribution of SO_2, NO_X, and O_3 over Secunda. This data is part of the data that was collected over Secunda in the morning on 18/03/2005 during the autumn campaign. The data was collected at approximately 167 magl flight level.

The uneven distribution of SO_2 concentration in space can be clearly seen in Figure 4.1. SO_2 concentration ranges between 0-6 ppb, with 28% frequency of occurrence. It was followed by the 18.1-24 ppb concentration range, with 18% frequency of occurrence. The remaining concentration ranges had a frequency of occurrence of +/- 10%. The concentration ranges of higher concentration had the least frequency of occurrence. This uneven spatial distribution of SO_2 could lead to disagreements between airborne and surface air quality data (Luke *et al*., 1998).

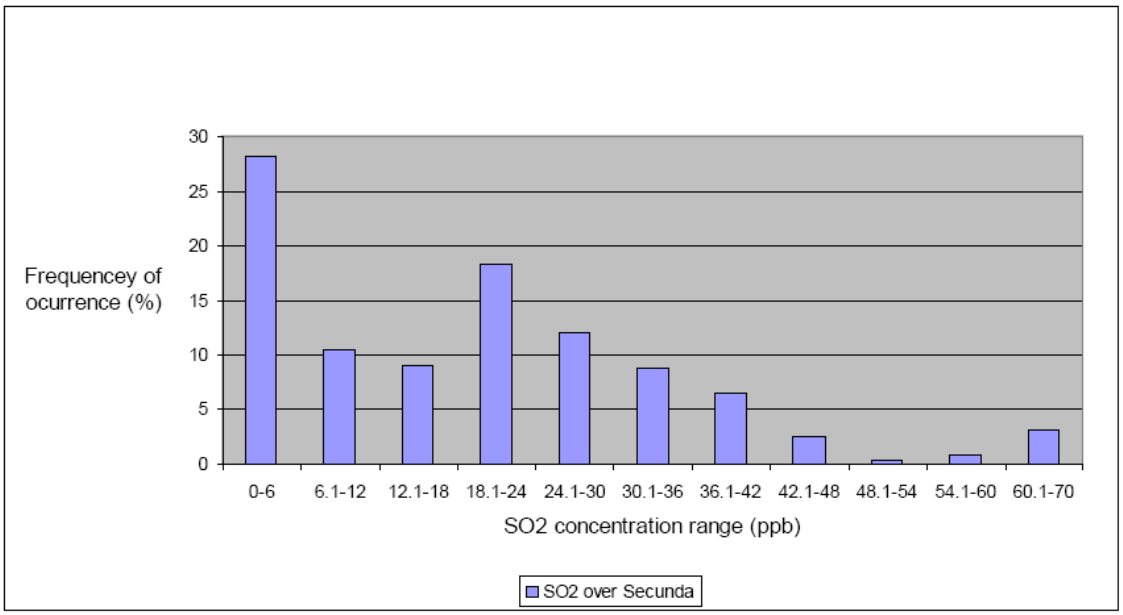

Figure 4.1: SO_2 concentration frequency distribution over Secunda at approximately 167 magl during the autumn campaign.

The uneven distribution of NO_X concentration in space can also be seen in Figure 4.2. The majority of the NO_X data were lying within the concentration range 1.1-2 ppb, with 17% frequency of occurrence. It was followed by the 0-1 ppb and 8.1-9 ppb concentration ranges, both with 9% frequency of occurrences. Then the 2.1-3 ppb and 3.1-4 ppb concentration ranges, both with 8% frequency of occurrences. The remaining concentration ranges had a frequency of occurrence that was less than 6%. This spatial variation of NO_X concentration can also lead to poor comparison of airborne and surface air quality data (Luke *et al*., 1998).

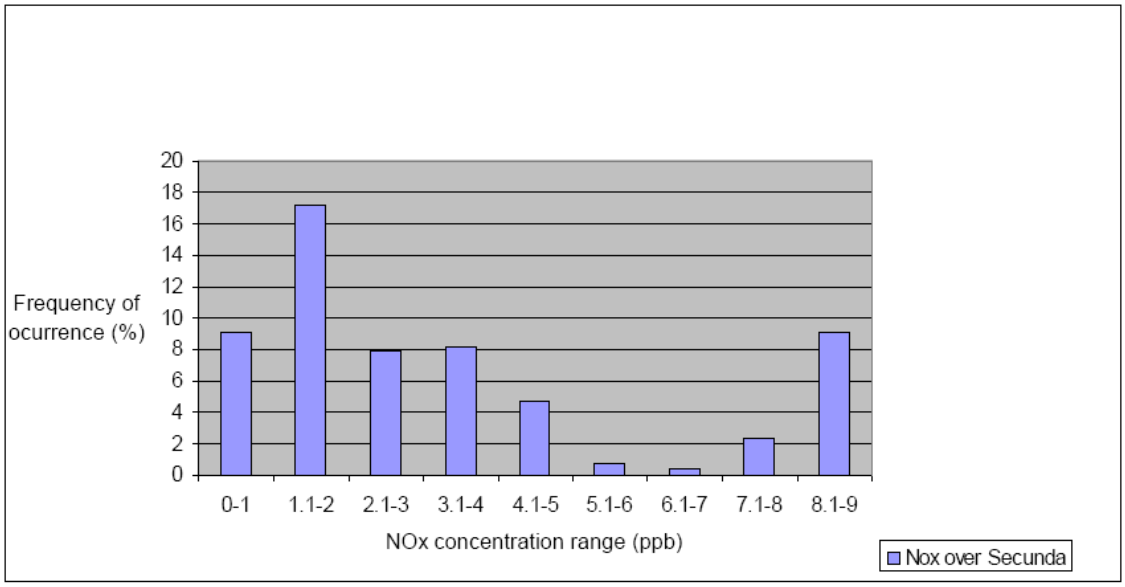

Figure 4.2: NO_X concentration frequency distribution over Secunda at approximately 167 magl during the autumn campaign.

In comparison to SO_2 and NO_X in Figure 4.1 and 4.2 respectively, Figure 4.3 shows that O_3 concentration varied the least in space. O_3 is a relatively long lived air pollutant, hence it has more time to mix and become uniformly distributed in space (Luke *et al*., 1998; WMO, 2006). Most of the O_3 concentration was within the concentration range 32.1-40 ppb, with 37.5% frequency of occurrence. It was followed by the 24.1-32 ppb concentration range, with 24% frequency of occurrence. Then the 16.1-24 ppb concentration range, with 20.6% frequency of occurrence. The remaining concentration ranges of higher concentrations had frequency of occurrences of about 2%. The relative uniform distribution of O_3 in space in comparison with SO_2 and NO_X is also confirmed by the relative standard deviation of these air pollutants at 167 magl flight level (Table 4.1). The relative uniform distribution of O_3 in space is a favourable condition for comparing airborne and surface measurements of this pollutant (Luke *et al*., 1998).

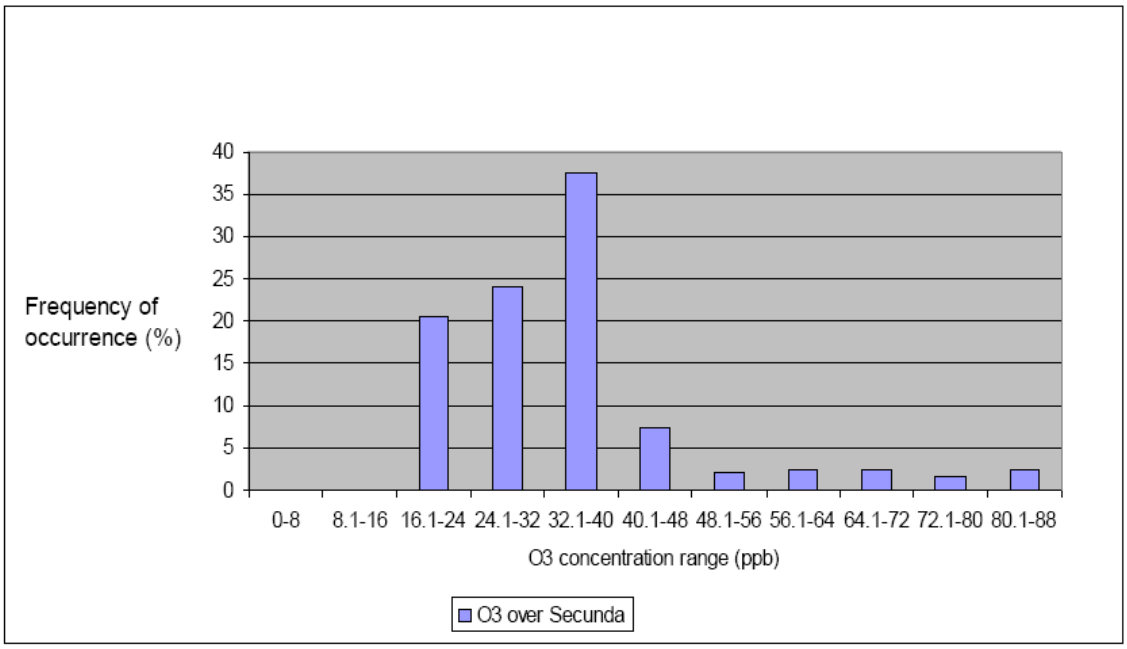

Figure 4.3: O_3 concentration frequency distribution over Secunda at approximately 167 magl during the autumn campaign.

Air pollution source height levels

Figure 4.4 shows the data that was collected in the morning along the boundaries of the Vaal Triangle during the air pollution flux provincial cross boundary campaign. The data was collected on 31/03/2006 during vertical profile flights of up to 3 km altitude. Irene weather observation station midday upper air data was also used to complement the temperature vertical profile from the aircraft. The data generated from this campaign is used to show the vertical uneven distribution of pollutants caused by the release of fresh emissions at different heights.

The temperature vertical profiles in Figure 4.4(a) and Figure 4.4(b) from both platforms; the aircraft and balloon-borne radiosonde, show an unstable lower column of the troposphere. However the SO_2 concentration vertical profiles in Figure 4.4(a) and Figure 4.4(b) show two bands of SO_2 plumes at different altitudes. Figure 4.4(a) shows 48.4 ppb and 26 ppb SO_2 concentration peaks at 1720 masl and 2000 masl respectively. Figure 4.4(b) shows 27.6 ppb and 5.4 ppb SO_2 concentration peaks at 1864 masl and 2688 masl respectively. This vertical gradient in SO_2 concentration distribution is caused by fresh emissions of air pollutants at different heights (Luke *et al*., 1998). Both the

Vanderbijlpark and Denesyville SO_2 vertical profiles have a peak close to the surface and another at a higher altitude. This variation of SO_2 concentration in the vertical leads to poor comparison of airborne and surface air quality data for this pollutant (Luke *et al.*, 1998).

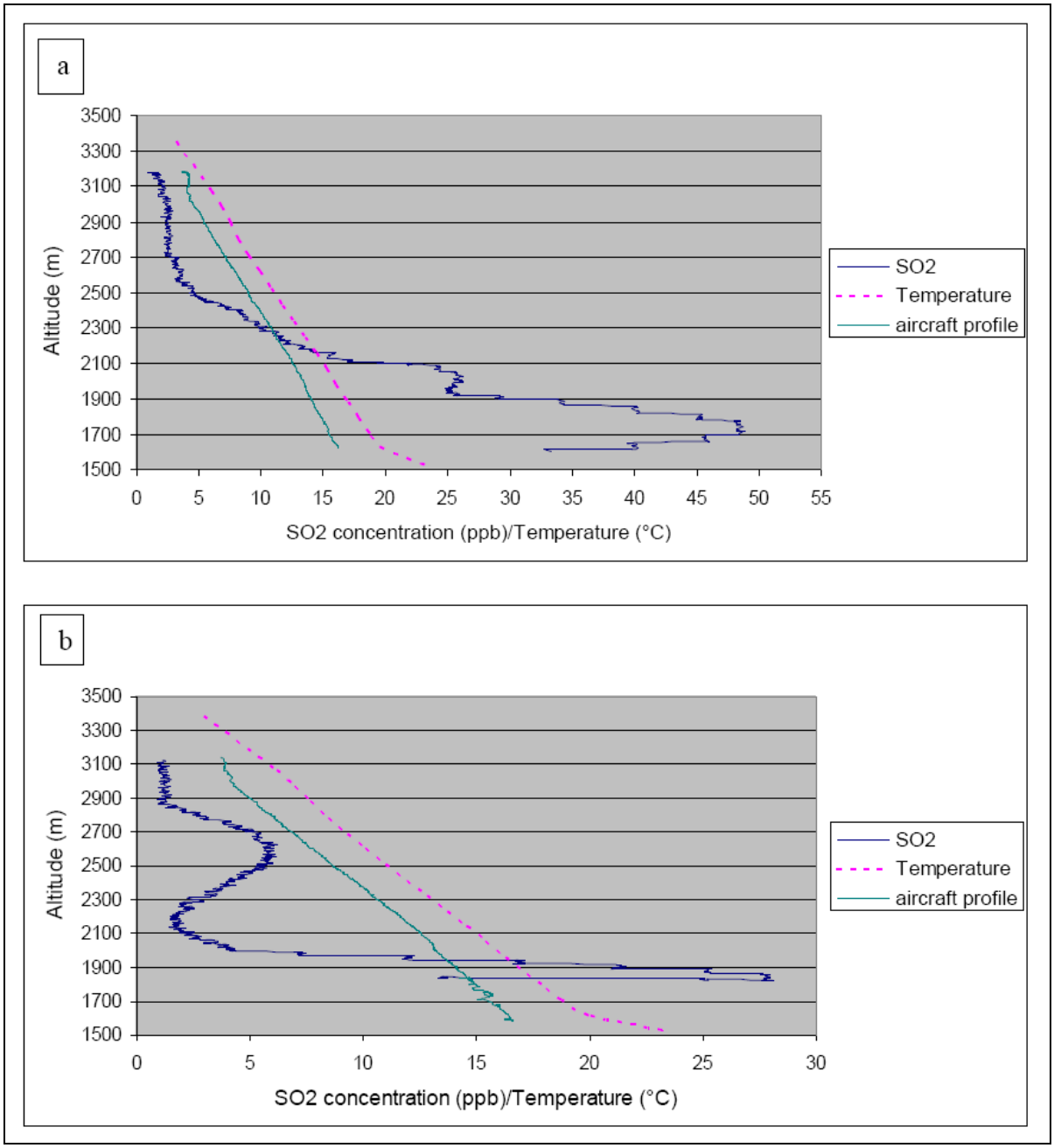

Figure 4.4: SO_2 and temperature vertical profiles. The dotted line on both Figures 4.4(a) and 4.4(b) are temperature profiles measured over Irene weather station and the SO_2 and the other temperature profiles are measured from the aircraft. Figure 4.4(a) is a vertical profile over Vanderbijlpark, Figure 4.4(b) is a vertical profile over Denesyville.

Direct comparison of airborne against ground based air quality data

The Figures 4.5 and 4.6 show the comparisons of SO_2 and O_3 of ground based data against airborne data. The ground based data are a one hour averaged data from Sasol and Mittal Steel air pollution monitoring sites. Airborne data were collected in a vicinity of these ground based air pollution monitoring sites. The airborne data measurement is instantaneous and the data were collected when the aircraft was flying within a 20 km radius from the ground based monitoring sites. Because of the unavailability of high resolution temporal ground based data. Airborne data were compared with an hour average and the month average of that specific hour that correspond to a time the aircraft flew within 20 Km radius from a ground station. The variability of the ground based data was determined by calculating the monthly standard deviations, using a specific hour that correspond to a time the aircraft flew within 20 Km radius from a ground station. The observations were made during the autumn and winter field campaigns. Table 4.3 shows the times and the altitudes at which the air pollutants in Figure 4.5 and 4.6 were monitored by both platforms.

The comparisons between airborne and surface hourly measurements of SO_2 in Figure 4.5 are not as close as the comparisons of O_3 measurements from the two monitoring platforms which are almost exact (Figure 4.6). The difference between the comparisons of airborne and ground based measurements of SO_2 and O_3 can be explained by a number of factors. To begin with the two data sets are being averaged over different temporal scales. The ground based data is averaged over an hour and the airborne data is an instantaneous data (averaged over a second). The uneven spread of SO_2 sources in space over the study sites (Wells, 1996) cause an uneven spatial distribution of SO_2 concentrations. This spatial variation of SO_2 levels is established in Figure 4.1. Relative standard deviations in Table 4.1 and Table 4.2 also show that SO_2 is more variable in space than O_3 at all flight levels monitored. The emission of SO_2 at different heights over the study sites (Wells, 1996) creates a vertical concentration gradient in their vertical distribution (Luke *et al*., 1998). Figure 4.4(a) and Figure 4.4(b) show this vertical concentration gradient caused by fresh emissions from different source heights, even

though the lower troposphere was unstable and well mixed. The relatively short atmospheric lifetime of SO_2 (one week) in comparison with O_3 (28 days) (Luke *et al*., 1998; Seinfeld and Pandis, 2006) results in smaller spatial extent of higher concentrations of SO_2 (Annegarn *et al*., 1996a), which in turn leads to spatial variation of SO_2. The vertical and horizontal variation of SO_2 caused by the above mentioned factors, reduces the extent of agreement between airborne and surface monitored air quality data.

Figure 4.5 show that the hourly SO_2 ground station data at Langverwatch and Bojesspriut is twice the levels monitored by the aircraft. The hourly SO_2 ground based data at Opsis 350 and Opsis 620 are relatively comparable to aircraft data. The monthly standard deviations for all ground stations show that SO_2 is temporarily highly variable. The standard deviations for SO_2 airborne data are small and close to zero. This is because the data extracted within 20 Km radius from ground stations are few values measured within short distances and times. Data measured within a short distance away from sources can be relatively uniform.

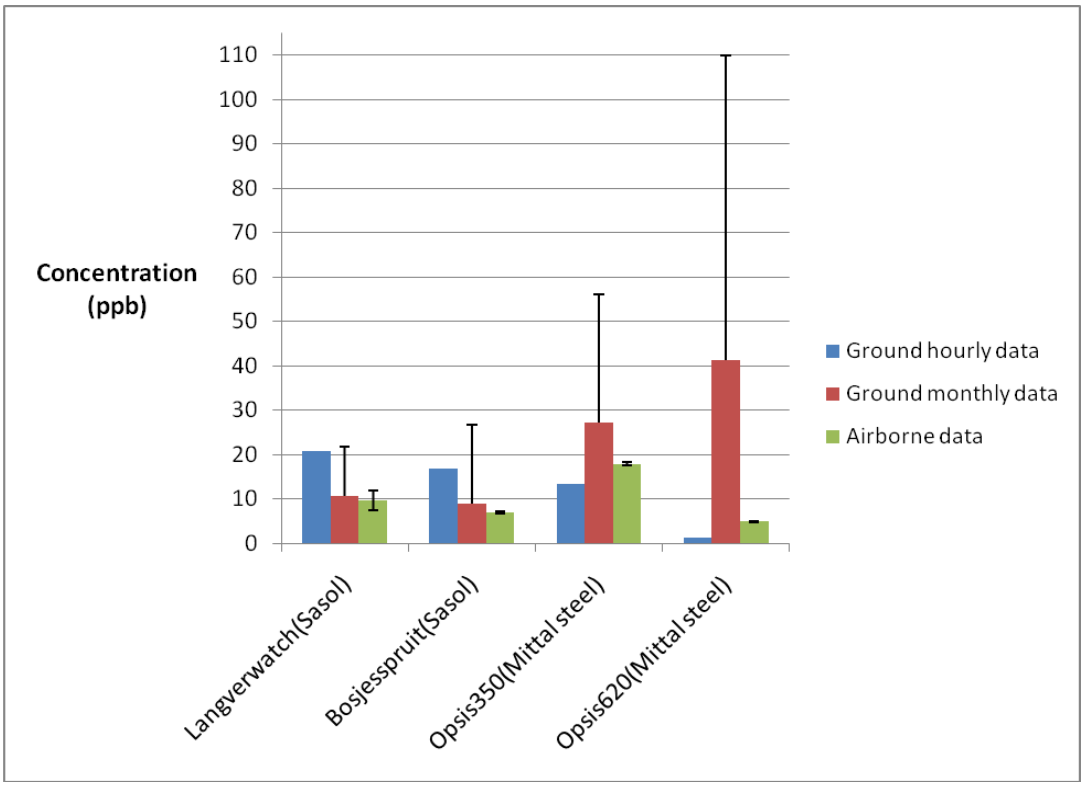

Figure 4.5: Direct comparison of airborne and ground based measured SO_2 data.

The comparisons between airborne and surface measured O_3 in Figure 4.6 show some relative good agreements. O_3 is a secondary air pollutant with a relatively long atmospheric lifetime (28 days). This characteristic of O_3 affords it more opportunity to be uniformly distributed in space as compared to short lived pollutants like SO_2 and NO_X (Luke *et al.*, 1998). The smaller variation in space of O_3 can be seen in Figure 4.3. Relative standard deviations of O_3 in Table 4.1 and Table 4.2 derived from morning and afternoon monitoring respectively, show that O_3 is more uniformly distributed in space and the comparable O_3 average concentrations at different flight levels suggests uniformity in vertical as well. This relative uniformity in space of O_3 explains the good comparison of the two data sets. Monthly standard deviations for Leitrim ground station show that O_3 is temporarily less variable. This explains the relatively good agreements between the O_3 hourly ground data and instantaneous airborne data. Standard deviations for airborne data were small and zero at some instances. This is due to the same reason already given in the case of SO_2 airborne data.

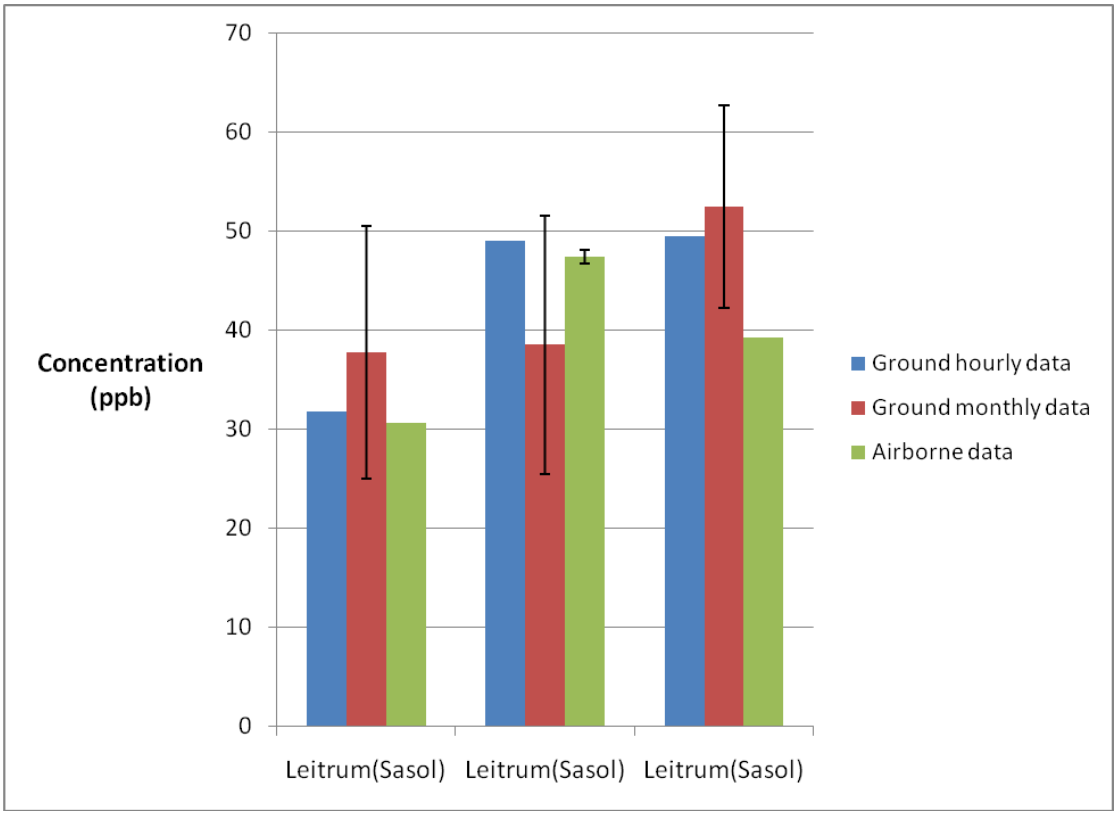

Figure 4.6: Direct comparison of airborne and ground based measured O_3 data.

Table 4.3: The times and altitudes at which SO_2 and O_3 were monitored by the aircraft and ground air quality monitoring stations.

Date	Time (SAST)	Campaign	Monitoring platform	Altitude (m)	Pollutant
17/03/2005	17:00:00	Autumn	Opsis 350 (Mittal Steel)	Ground	SO_2
17/03/2005	16:44:40	Autumn	Opsis 350 (airborne)	1735.71	SO_2
17/03/2005	16:00:00	Autumn	Opsis 620 (Mittal Steel)	Ground	SO_2
17/03/2005	15:58:37	Autumn	Opsis 620 (airborne)	1673.86	SO_2
18/03/2005	11:00:00	Autumn	Langverwatch (Sasol)	Ground	SO_2
18/03/2005	10:28:00	Autumn	Langverwatch (airborne)	1604.96	SO_2
18/03/2005	13:00:00	Autumn	Bosjesspruit (Sasol)	Ground	SO_2
18/03/2005	12:46:00	Autumn	Bosjesspruit (airborne)	2385.28	SO_2
21/07/2005	15:00:00	Winter	Leitrim (Sasol)	Ground	O_3
21/07/2005	14:41:30	Winter	Leitrim (airborne)	1270.00	O_3
25/07/2005	14:00:00	Winter	Leitrim (Sasol)	Ground	O_3
25/07/2005	14:17:00	Winter	Leitrim (airborne)	1632.18	O_3
03/08/2005	15:00:00	Winter	Leitrim (Sasol)	Ground	O_3
03/08/2005	14:42:34	Winter	Leitrim (airborne)	1673.50	O_3

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Factors influencing mixing in the troposphere, which in turn influences the agreement between airborne and surface monitored air quality data, were considered in this chapter. The diurnal evolution of the mixing layer plays an important role in the agreement between airborne and surface air quality data. Uneven spatial distribution of air pollutants sources, with different temporal emission cycles can lead to disagreements between airborne and surface air quality data. The atmospheric lifetime of air pollutants also complicates the comparison of the two data sets. O_3 an air pollutant with a relatively long atmospheric lifetime gives good comparison of the two data sets, and SO_2 a highly variable pollutant in space and time with a short atmospheric lifetime gives less agreements between the two data set.