SP-1196 (6)

REPORTS FOR ASSESSMENT

THE NINE CANDIDATE EARTH EXPLORER MISSIONS

Atmospheric Chemistry Mission

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Atmospheric Chemistry Mission

ESA SP-1196 (6) – The Nine Candidate Earth Explorer Missions –
ATMOSPHERIC CHEMISTRY MISSION

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1. Introduction

For the post 2000 time frame two general classes of Earth Observation mission have been identified to address user requirements, namely:

> **Earth Explorer Missions** – these are research/demonstration missions with the emphasis on advancing understanding of the different processes which help govern the Earth system. The demonstration of specific new observing techniques also comes under this category.
>
> **Earth Watch Missions** – these are pre-operational missions addressing the requirements of specific application areas in Earth Observation. The responsibility for such missions would be transferred eventually to operational (European) entities and to the private sector.

Nine Earth Explorer missions have been identified as potential candidates for Phase A study and a Report for Assessment has been produced for each of these candidate missions.

This particular Report for Assessment is concerned with the Earth Explorer Atmospheric Chemistry Mission. It has been prepared by one of the nine Mission Working Groups that have been established to produce these Reports. The four (external non-ESA) members of this particular Group are I. Isaksen (University of Oslo, Oslo, Norway), G. Brasseur (Service d'Aeronomie du CNRS, Verrières-le-Buisson, France), B. Carli (IROE/CNR, Florence, Italy) and H. Kelder (KNMI, De Bilt, The Netherlands). They were supported by members of the Executive who advised on technical aspects and took the lead in drafting technical/ programmatic sections. This Report, together with those for the other eight candidate Earth Explorer Missions, is being circulated amongst the Earth Observation research community in anticipation of a Workshop to be held in Spain in May 1996.

This mission recognises the need to focus on the chemistry of the upper troposphere/ lower stratosphere accepting the need to investigate the exchange of trace gases (in particular water vapour and ozone), as well as radiative and kinetic energy, between these two regions i.e. stratospheric/tropospheric exchange.

In the stratosphere it is expected that current high levels of chlorine and bromine loading will peak early in the next century. It is thus extremely important to pursue on-going efforts to quantitatively advance understanding of the changes in ozone and temperature which are expected to occur on this time scale. In so doing full account must also be taken of a) changes arising from increases in the concentrations of tropospheric gases, b) the radiative energy balance at the tropopause level and c) the dynamical structure of the lower stratosphere/ upper troposphere.

In the troposphere continuous increases are expected in the concentrations of the precursors of tropospheric ozone and in the greenhouse gases. Aerosols, from both natural and anthropogenic sources, can be expected to play an increasing role in the chemistry of the troposphere. Thus, on the post 2000 time frame, it will be necessary to a) accurately determine the changes in the oxidizing properties of the troposphere and in radiative forcing, both at the surface and at the tropopause and b) to advance knowledge of the chemical processes involved, in particular those controlling the life times of greenhouse gases.

All the Reports for Assessment follow a common structure comprising seven chapters. They each start by addressing the scientific justification for a particular mission and move on to detail its specific objectives. This is followed by a detailing of the specification of observation requirements and a listing of the various mission elements required to satisfy the observational requirements. Then consideration is given to the implications of meeting the observational requirements in terms of both the space and ground segment as well as requisite advances in scientific algorithms and processing/assimilation techniques. Finally programmatic aspects are considered.

2. Background and Scientific Justification

2.1. Introduction

Recent international assessments of ozone (WMO, 1995) and climate (IPCC, 1995) have served to highlight the importance of ozone on climate-chemistry interactions and of research on this subject. Furthering understanding of the chemistry of ozone is clearly necessary to advance our ability to interpret and predict its variability and its interaction with radiation in the atmosphere.

The ESA Chemistry Review Panel (ESA, 1995) identified two key regions of the atmosphere where further observations are vital for improving understanding. These are the upper troposphere (UT) and the lower stratosphere (LS). The discussion in this Report therefore focuses on this part of the atmosphere where the deficiencies in our knowledge relate not only to the global distribution of ozone and the changes in its concentration but also to the key compounds involved in its formation and loss. Global, high resolution, observations of chemical compounds by satellites could provide information on the global distribution of these key compounds.

In the following two sub-sections the outstanding problems are summarised, while the current state of understanding is reviewed in sections 2.2 to 2.5 leading to a discussion of possible contributions of satellite observations to the study of atmospheric chemistry (section 2.6).

2.1.1. Stratospheric Ozone Depletion

Large decreases in ozone have been recorded over the Antarctic for many years but, since 1991, significant ozone reductions have also been observed at Northern mid- and high-latitudes (Gathen et al., 1995). Figure 2.1 demonstrates the way the shortwave solar radiation (UV-B) is anti-correlated with the ozone column density. It is clear that there has been a significant increase in levels of shortwave solar radiation (including UV-B) during the time period 1991 through 1993 at Northern latitudes when observations showed a particularly large decrease in ozone column densities.

The main cause of the observed ozone reductions since 1980 is the anthropogenic emission of trace species into the atmosphere, notably the chlorofluorocarbons (CFCs), which produce free chlorine in the LS and the halons as a source of bromine radicals. The main ozone losses have occurred in the LS at heights below (approximately) 25 km (WMO, 1995). The levels of two of the major contributors to stratospheric chlorine loading, namely CFC-11 and CFC-12, are already starting to show reduced growth due to the implementations of regulations aimed at reducing their emissions, and these levels are expected to start to decline within the next decade. It will be of particular importance to follow (and interpret) the impact of these changes on the levels of chlorine and bromine compounds in the stratosphere, and to observe how the ozone depleting process develops over the next one to two decades.

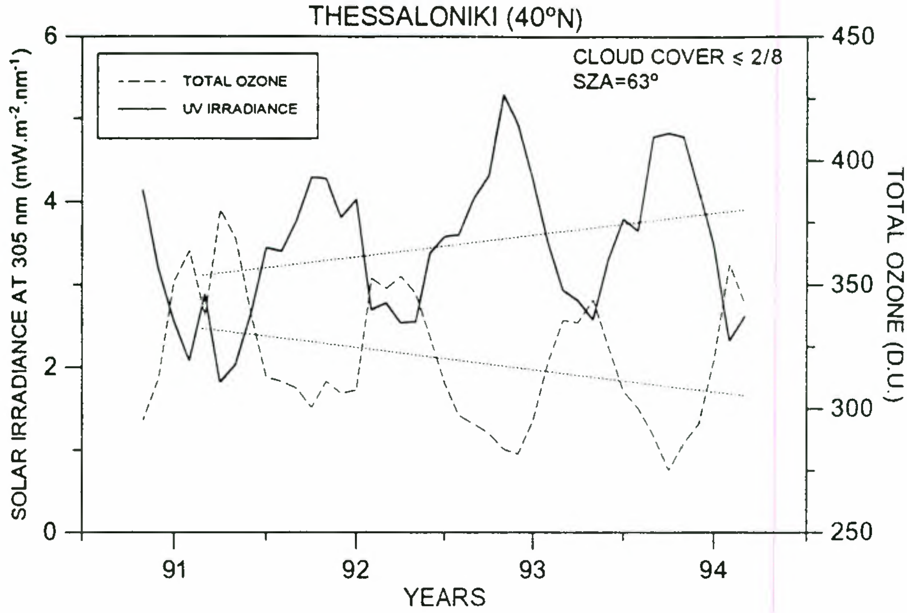


Figure 2.1. Variation of monthly mean monochromatic solar flux in the UV-B spectral region (305 nm) and corresponding total ozone change during the period from 1991 to 1994 (Zerefos, 1995).

2.1.2. Climate-chemistry Interactions

Long term changes in the Earth's climate, caused by changes in the abundances of radiatively active compounds in the atmosphere, are expected to become significant during the first half of next century (IPCC, 1995). Increases in the concentrations of several of the known radiatively active compounds have already contributed to the increase in global mean radiative forcing since pre-industrial times. This is illustrated in figure 2.2 and it can be seen that the largest contribution to these observed changes is associated with the increase in the concentration of carbon dioxide (water vapour is a special case as discussed in section 2.4). However, it is also clear that changes in the concentrations of radiatively active species, such as methane, nitrous oxide, the CFCs and ozone, have together contributed to approximately 30–40% of the observed global average radiative forcing since 1850 (IPCC, 1995).

Ozone is of particular importance when viewed in the context of chemistry-climate interactions. Changes in its distribution will have the largest impact on surface temperatures when changes occur in the LS and the UT (Wang et al, 1980) and it is pertinent to note that, over the last two decades, observations show that ozone concentrations have fallen in the LS and increased in the UT. The depletion in stratospheric ozone levels has probably produced a general cooling of the climate system (figure 2.2) that may have partly counter-balanced the warming caused by increases in the CFCs, other halocarbons and tropospheric ozone. However, these two effects cannot be directly compared, because the spatial patterns associated with radiative forcing by ozone and by the well mixed greenhouse gases are very different.

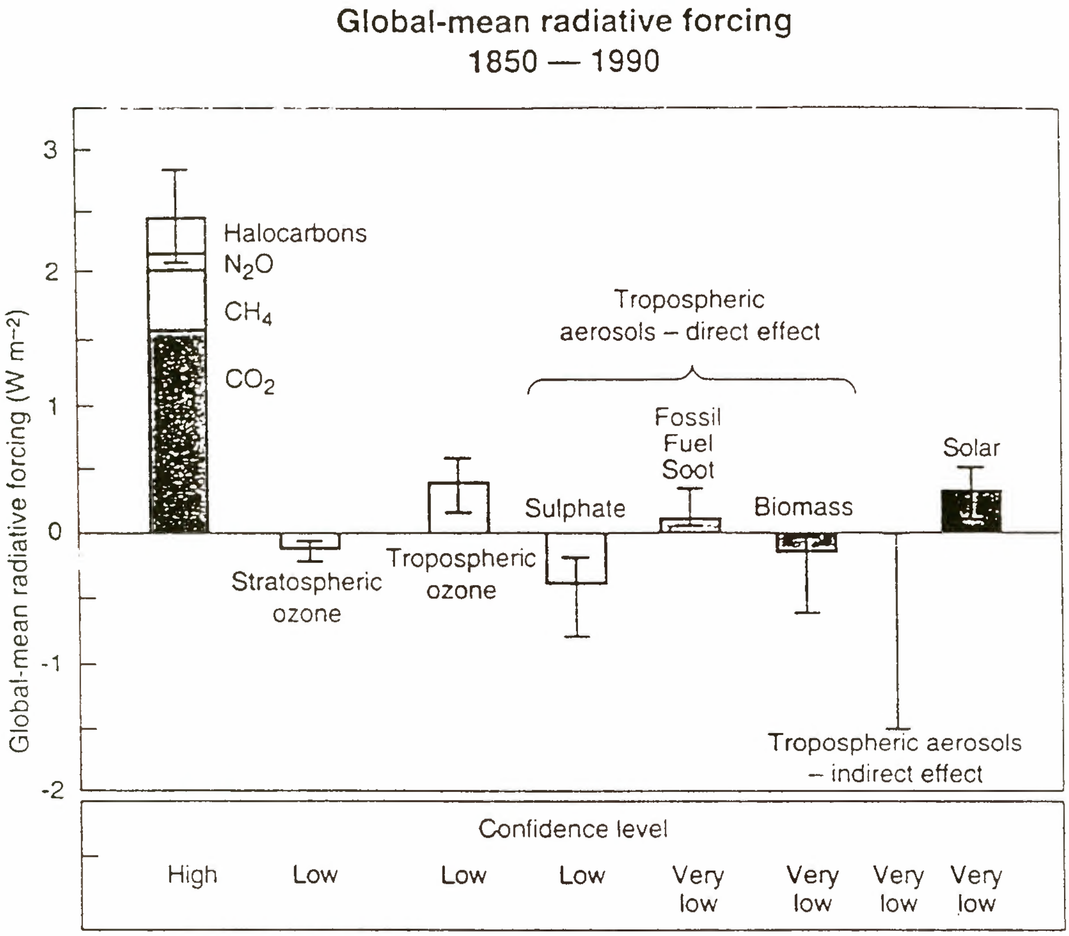


Figure 2.2. Estimates of the globally averaged radiative changes due to changes in greenhouse gases and aerosols from preindustrial times to the present day and changes in solar flux from 1850 to the present day. An indication of relative confidence in the estimates is given below each bar (IPCC, 1995).

The impact on radiative forcing associated with increases in tropospheric ozone will be regional in character. Hauglustaine et al. (1994) have shown (see figure 2.3) that ozone has been the second (after carbon dioxide) most important contributor to radiative forcing at the Northern hemispheric mid-latitudes, where the abundance of ozone is believed to have increased most as a result of anthropogenic activities. Another important point is the probable coupling between climate and ozone depletion in the LS through reduced temperatures which are likely to enhance ozone loss through more frequent polar stratospheric cloud (PSC) formation. A large fraction of the temperature trends observed globally in the LS over the last two decades (figure 2.4) could be associated with ozone depletion.

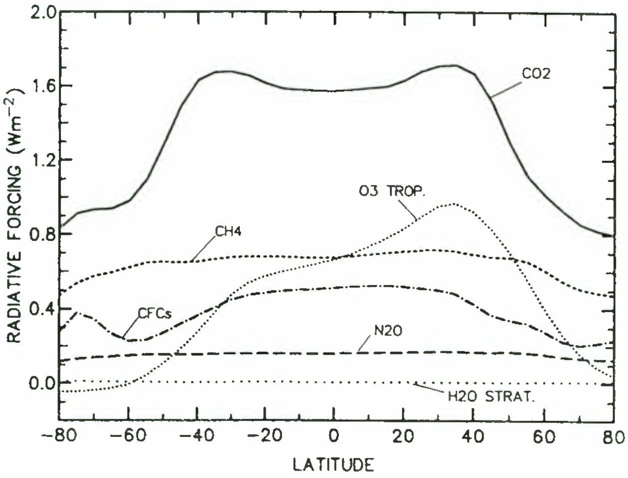


Figure 2.3. *Latitudinal dependence of the calculated 'surface to troposphere' annually averaged radiative forcings due to greenhouse gas increases since preindustrial time (Hauglustaine et al., 1994).*

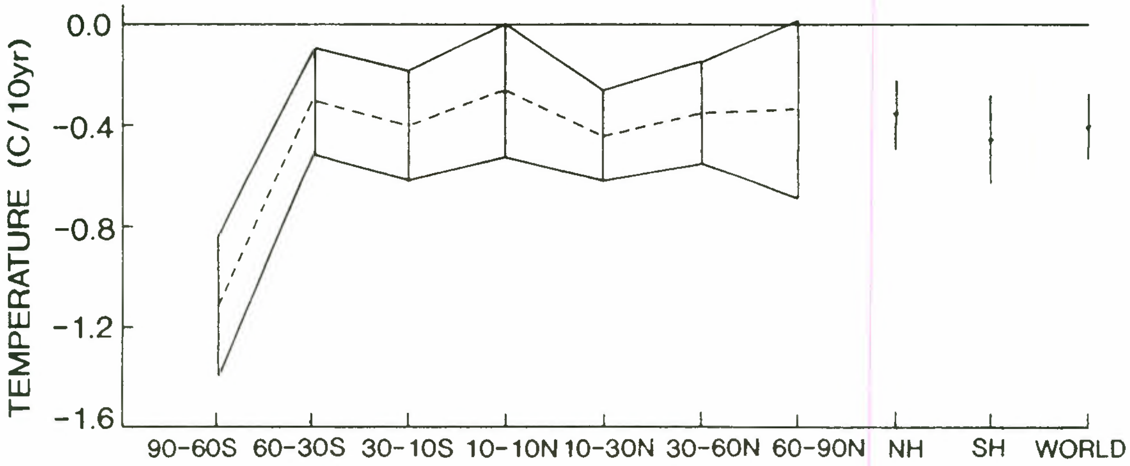
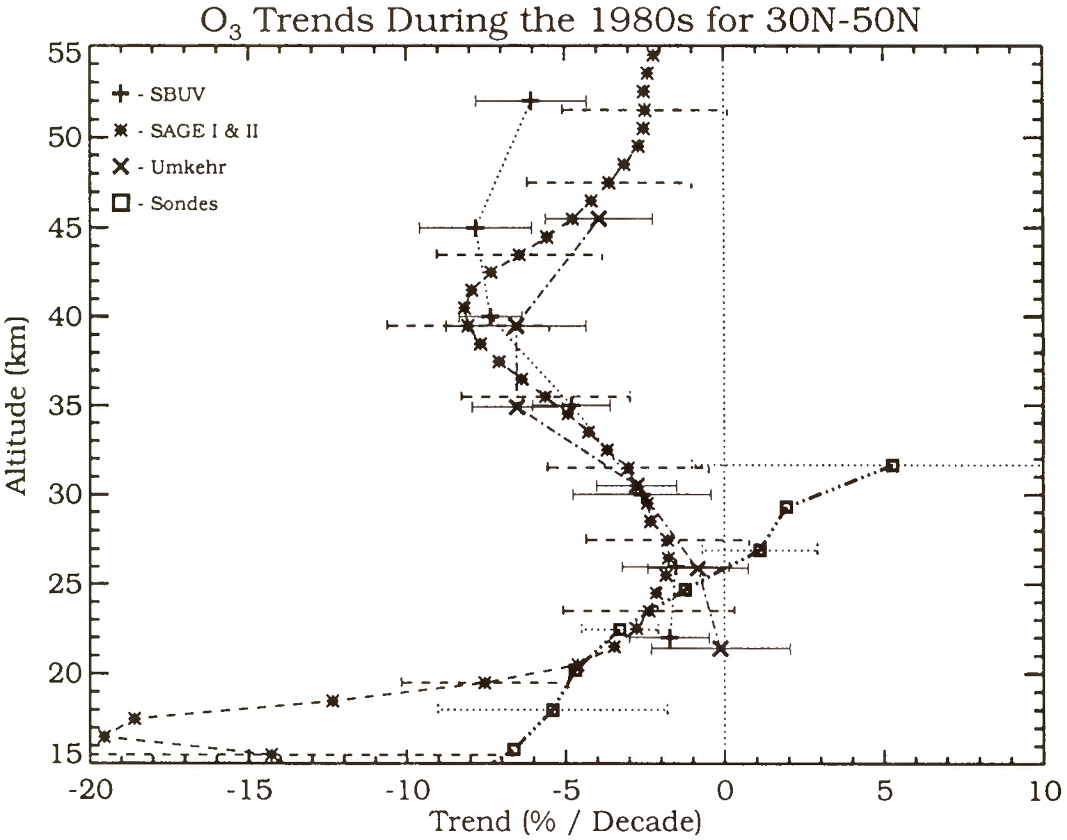


Figure 2.4. *Latitudinal variations of estimated trends in annual mean temperatures (in deg C / decade) from radiosonde analysis for the 100–50 hPa layer during the period December 1963 to November 1989. The 95% confidence limits are also shown (WMO, 1995).*

2.2. Ozone Chemistry

Observations indicate that largest decreases in ozone have occurred in the LS (figure 2.5) and, one of the major needs, which is a prerequisite for progress in our understanding of the processes that affect the distribution of ozone in the UT and LS, is to obtain a global ozone climatology of this region of the atmosphere. An equally important (and closely linked) task is to quantify the contributions from the different processes affecting the ozone budget in this region. This necessitates the observation of other species in addition to ozone itself (see later).



2.5. Trends in the vertical distribution of ozone during the 1980s from satellite, sonde and Umkehr observations (WMO, 1995).

In general ozone loss is caused by catalytic destruction which takes the following general form:

$$
\begin{array}{lllll}
X & + & O_3 & \rightarrow & XO & + & O_2 \\
XO & + & O & \rightarrow & X & + & O_2 \\
\hline
O & + & O_3 & \rightarrow & 2O_2 & &
\end{array}
$$

where X = NO_x, HO_x etc. However, the actual processes involved vary from one part of the atmosphere to another, as does the level of understanding.

2.2.1. Ozone Chemistry in the Lower Stratosphere

The major ozone loss in the LS at high latitudes is associated with the following catalytic cycle involving chlorine:

$$\begin{array}{llllllllll}
ClO & + & ClO & + & M & \rightarrow & Cl_2O_2 & + & M & \\
Cl_2O_2 & + & h\nu & & & \rightarrow & Cl & + & ClO_2 & \\
ClO_2 & & & & & \rightarrow & Cl & + & O_2 & \\
2(Cl & + & O_3) & & & \rightarrow & 2(ClO + O_2) & & & \\
\hline
O_3 & + & O_3 & & & \rightarrow & O_2 & + & O_2 & + \; O_2
\end{array}$$

where ‘M’ represents an arbitrary particle picking up the momentum set free by the reaction and hν indicates the impact of radiation.

As the loss of ozone is proportional to the square of the concentration of ClO the cycle becomes efficient in areas with high concentrations of ClO (i.e. areas where the chemistry is strongly affected by heterogeneous reactions on PSCs).

Additional loss occurs via reactions involving chlorine and bromine oxides:

$$\begin{array}{lllllllll}
BrO & + & ClO & \rightarrow & Br & + & Cl & + & O_2 \\
Br & + & O_3 & \rightarrow & BrO & + & O_2 & & \\
Cl & + & O_3 & \rightarrow & ClO & + & O_2 & & \\
\hline
O_3 & + & O_3 & \rightarrow & O_2 & + & O_2 & + & O_2
\end{array}$$

as well as by reactions involving hydrogen:

$$\begin{array}{lllllllll}
BrO & + & HO_2 & \rightarrow & HOBr & + & O_2 & & \\
HOBr & + & h\nu & \rightarrow & Br & + & OH & & \\
Br & + & O_3 & \rightarrow & BrO & + & O_2 & & \\
\hline
O_3 & + & HO_2 & \rightarrow & O_2 & + & O_2 & + & OH
\end{array}$$

Ozone destruction by chlorine is reduced by the formation of HCl:

$$Cl + CH_4 \rightarrow HCl + CH_3$$

Another reaction of large importance in this part of the atmosphere is the interaction of chlorine and nitrogen compounds:

$$ClO + NO_2 + M \rightarrow ClONO_2 + M$$

This reaction reduces concentrations of active chlorine and nitrogen compounds and thereby the efficiency of catalytic ozone destruction by chlorine and nitrogen.

Heterogeneous chemistry (on PSCs and sulphate aerosols) also plays a key role by converting stable reservoir gases to active ozone reducing gases:

$$\begin{array}{lllll}
ClONO_2 & + HCl & \rightarrow & Cl_2 & + & HNO_3 \\
ClONO_2 & + H_2O & \rightarrow & HOCl & + & HNO_3 \\
N_2O_5 & + HCl & \rightarrow & ClNO_2 & + & HNO_3 \\
N_2O_5 & + H_2O & \rightarrow & HNO_3 & + & HNO_3 \\
HOCl & + HCl & \rightarrow & Cl_2 & + & H_2O
\end{array}$$

The products of these heterogeneous reactions (i.e. Cl_2, HOCl and $ClNO_2$) are easily dissociated by solar radiation. Another consequence of the above reactions is the conversion of nitrogen compounds to the more stable HNO_3.

Although the chemistry discussed above is most active in the Antarctic and Arctic regions in winter and early spring, its role at mid-latitudes (particularly the reactions involving bromine compounds) could also be significant, especially after large volcanic eruptions (e.g. Mt. Pinatubo in 1991) when the particle loading of the LS can be enhanced by more than a factor ten (e.g. WMO, 1995). Variations in the levels of PSCs and volcanic particles lead to large variations in chemical activity (and hence ozone loss) in the LS.

To understand the processes discussed above requires global (and simultaneous) observations of the key chemical compounds at a spatial resolution sufficiently high to explore the large variability of the atmosphere. In particular, the measurement of ClO concentrations in the LS is crucial for the estimation of ozone loss in this part of the atmosphere. Several airborne campaigns (e.g. from the NASA ER-2) have shown that, in air masses affected by PSCs, the mixing ratio of ClO can exceed 1 ppbv and, further, that large amounts of ozone are destroyed in such regions. Observations of the distribution of ClO, with mixing ratios consistent with the airborne observations, have been provided by the MLS instrument on board UARS (though the accuracy of these data are not adequate to provide the required insights into the requisite chemical processes).

A thorough study of the mechanisms involved in ozone destruction in the LS requires knowledge of the global distribution of chlorine reservoirs as well as that of the nitrogen oxides (which closely interact with chlorine compounds). In order to quantify the total amount of inorganic chlorine present in the stratosphere, it would also be necessary to observe the abundances of HCl and probably $ClONO_2$ in the stratosphere. The reduction of the uncertainties will be of particular importance beyond year 2000, a period when levels of chlorine are expected to decrease as a result of the implementation of the Montreal Protocol and its amendments.

2.2.2. Ozone Chemistry in the Troposphere

In the free troposphere (as in the LS) the chemistry is initiated by the photodissociation of ozone:

$$O_3 + h\nu \rightarrow O(1D) + O_2$$

followed by the oxidation of water vapour:

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

These are key chemical reactions in initiating the oxidation process. This means that the presence of solar radiation in the UV-B region (where the dissociation takes place) and water vapour are crucial for ozone production and ozone loss in this part of the atmosphere. Given the large variations in the concentration of water vapour that have been observed, it is critical to ensure a good global observation of its distribution and to determine how it is affected by stratospheric/tropospheric exchange processes. Variations in levels of UV-B radiation will also have a significant impact on the chemistry, particularly in the troposphere.

In the UT the initial reactions are followed by a large number of reactions which establish equilibrium between OH and HO_2 and which can lead to ozone loss or ozone production. A short description of key reactions is given below.

Conversion of OH to HO_2 occurs mainly through the reaction:

$$OH + CO\ (+O_2) \rightarrow HO_2 + CO_2$$

and through the oxidation of methane:

$$CH_4 + OH \rightarrow CH_3 + H_2O$$

leading to the formation of the hydroperoxy radicals (HO_2) and the organic peroxy radicals (RO_2).

Ozone is formed in the free troposphere through the sequence of reactions:

$$\begin{array}{llllllll} NO & + & HO_2 & & \rightarrow & NO_2 & + & OH \\ NO_2 & + & hv & & \rightarrow & NO & + & O \\ O & + & O_2 & + M & \rightarrow & O_3 & + & M \\ \hline O_2 & + & HO_2 & & \rightarrow & O_3 & + & OH \end{array}$$

Similar cycles, with the hydroperoxy radicals (HO_2) replaced by organic peroxy radicals (RO_2), also contribute to ozone formation, but they probably play a secondary role in the vicinity of the tropopause.

Chemical destruction of ozone in the free troposphere reflects the presence of hydroperoxy and hydroxyl (OH) radicals. The key reactions in ozone loss in the free troposphere are:

$$\begin{array}{llllll} HO_2 & + O_3 & \rightarrow & OH & + & 2O_2 \\ OH & + O_3 & \rightarrow & HO_2 & + & O_2 \end{array}$$

The photolysis of ozone followed the reaction with water vapour will also lead to the loss of ozone.

A full quantification of ozone production in this part of the atmosphere requires the determination of daytime concentrations of NO_x and HO_x.

So far only limited observations of the distribution of NO_x in the free troposphere have been made, and, as in the case of ozone observations, mostly in the Northern Hemisphere. The observations (mostly from surface stations) have shown that NO_x levels vary from a few tens of ppt in remote regions to in excess of ppb in industrial regions. Characteristic is the high spatial and temporal variability, which is a direct consequence of the short lifetime of NO_x and the very uneven distribution of sources of NO_x. These sources include combustion processes (energy consumption and biomass burning) and emissions from the surface, as well as lightning flashes and aircraft emissions directly into the atmosphere. In addition, vertical convective transport directly affects the distribution of NO_x in the UT. An important unknown in the budget of the NO_x is the rate at which it is recycled from nitrogen reservoirs such as HNO_3 and PAN (Peroxyl Acetyl Nitrate – assumed to be significant at middle and upper tropospheric levels). Even fewer observations exist of the concentrations of HO_2 and OH radical in this part of the atmosphere.

This question has to be addressed by global observations from space performed with adequate spatial resolution. If all involved species cannot be measured from space, the global behaviour could be characterised by space observations of suitable subsets of species in combination with model studies of ozone production and destruction and process oriented airborne campaigns.

2.3. Transport and Stratosphere/Troposphere Exchange

Dynamical, chemical and radiative coupling between the stratosphere and troposphere are among the important processes that must be understood if we are to provide an adequate description and prediction of global change. Of special significance is the exchange of chemical species (whether of natural or anthropogenic origin) between the stratosphere and the troposphere.

In the Atmospheric Chemistry Mission Report (ESA, 1995) the quantification of stratospheric-tropospheric exchange processes was identified as one of the key problems to be addressed by process-oriented satellite missions for the year 2000 and beyond. The insight that transport plays an important role in atmospheric chemistry is becoming more and more evident and is reflected in the 'state-of-the-art' atmospheric models which nowadays are three-dimensional containing an extensive description of chemistry as well as of dynamics. Uncertainties in the knowledge of some of the transport processes limit the performance of these models.

2.3.1. Different Modes of Transport

In transport a wide spectrum of scales are involved ranging from large scale ascent and descent, via synoptic scales, towards transport by waves, convection and turbulence (e.g.Brewer, 1949; McIntyre, 1992 and Holton et al., 1995). Here the focus is on the exchange between the troposphere and the LS (Hoskins et al., 1985). This part of the stratosphere is strongly coupled with the troposphere and is separated from the middle stratosphere by a region enclosed between the 380 K and 400 K potential temperature surfaces (see figure 2.6).

For the transport it is useful to distinguish between various different regions of the globe:

a) In the tropics it is mostly deep convection which takes care of upward transport, though smaller scale phenomena such as waves also play an important role. The tropics are the regions on Earth in which the largest net upward transport occurs and which therefore influence directly the composition of the global middle stratosphere.

b) In mid-latitudes the exchange between the troposphere and lowermost stratosphere is in both directions with a somewhat larger downward component (Siegmund et al. 1996). Most of this transport is related to the occurrence of extra-tropical cyclones and blocking anticyclones. In cyclones polar stratospheric air is sucked into the troposphere while subtropical tropospheric air is pushed into the stratosphere. The intermediate process of tropopause folding is followed by the re-establishment of the tropopause.

c) Around the polar vortices the exchange between the troposphere and stratosphere mostly occurs along isentropic surfaces, from the polar vortex towards mid-latitudes, by filaments torn off from the vortex boundary. Vertical transport in the vortex itself mostly takes place in the form of large scale descent by radiative cooling.

Quantitative knowledge of the various exchange mechanisms and their contribution to the chemistry of the stratosphere and troposphere is still lacking and to correct this deficiency and model the processes involved is one of the challenges to be faced in the next decade.

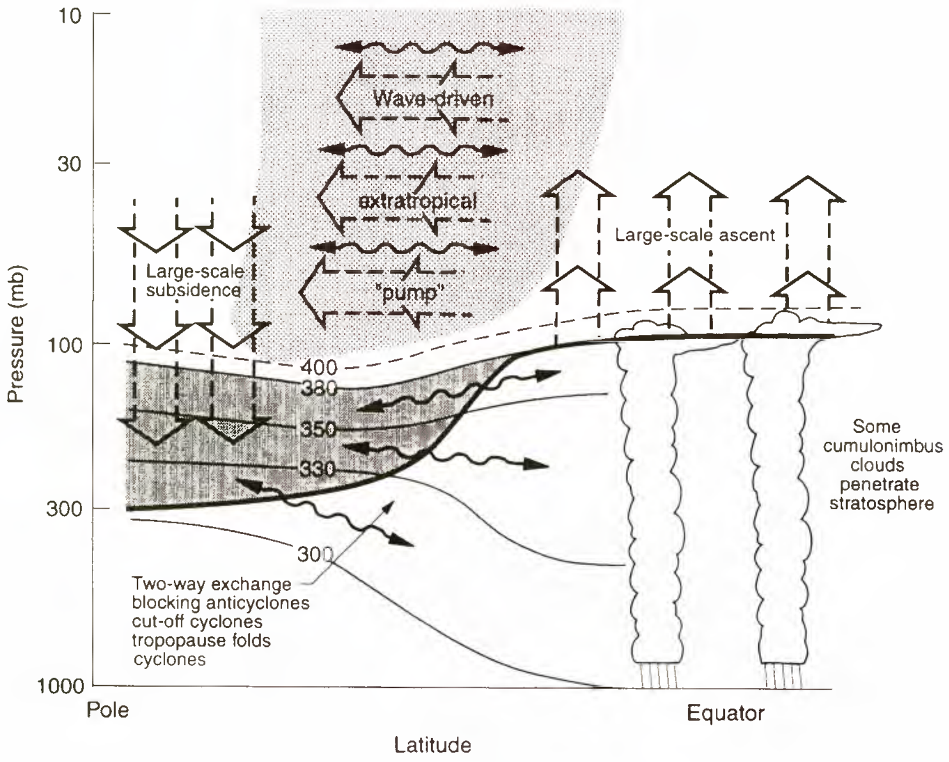


Figure 2.6. Dynamical aspects of stratospheric-tropospheric exchange. The tropopause is shown by the thick line. Thin lines denote isentropic or constant potential temperature surfaces labelled in Kelvin. The heavily shaded region represents the 'lowermost stratosphere', where isentropic surfaces span the tropopause and isentropic exchange by tropopause folding occurs. The region above the 380 K surface is the 'overworld', in which isentropes lie entirely in the stratosphere. Light shading in the 'overworld' denotes wave-induced forcing (the extratropical 'pump'). The wavy double-headed arrows denote meridional transfer by eddy motion. The broad arrows show transport by the global-scale circulation, which is driven by the extra-tropical pump (courtesy, Holton, 1995).

2.3.2. Representations of Transport and Stratospheric-Tropospheric Exchange in Models and Validation

Stratospheric/tropospheric exchange is a vital component of the general circulation of the atmosphere and must form part of the dynamical description contained in atmospheric models. Furthermore, the dynamics of the troposphere and stratosphere are inseparable (Hoskins et al., 1985) so models must include representation of both the troposphere and at least the lower parts of the stratosphere. Validation of the models have only been made on a very restricted basis and many unexplained discrepancies have been found.

This is not surprising as amongst other points the strong longitudinal asymmetries present in stratospheric/tropospheric exchange render current two-dimensional models inadequate. The provision of global data sets, coupled with the systematic assimilation of data into atmospheric models, offers the possibility of careful analysis of the three-dimensional model behaviour, both for longer (annual) timescales and shorter timescales associated with specific events. Only in this way will it be possible to advance understanding to the levels required.

2.3.3. Estimates of Global-Scale Exchange and Uncertainties

Part of the transport associated with stratospheric/tropospheric exchange can be observed by measuring changes in the distribution of certain species. Potential tracers for studying these upward transports include O_3, CO, N_2O, H_2O, CH_4 and SO_2. For downward transport O_3 is a representative indicator. The observations have to be made with rather high horizontal and vertical resolution as an important part of this transport takes place at quite small scales (van Velthoven and Kelder, 1996). Global data sets are needed to determine the global distribution of these processes and to reduce the current levels of uncertainty.

Thus, for example, current estimates of mass fluxes through the 100 Pa surface (about $50x10^8$ kgs^{-1} for the extra-tropical Northern Hemisphere), vary roughly by 50% between different authors (Holton et al., 1995). Estimates of ozone fluxes vary with a factor of two with a typical value of $6x10^{10}$ molecules per m^2 per second for the Northern Hemisphere. These estimates of the fluxes involved are mainly derived by extrapolating from events to global values and are consequently partly based on observations and partly on theoretical considerations.

The lack of knowledge of the magnitudes of various transport processes can have considerable impact on the estimates of the budgets of different trace gases and hence on our ability to model climate. For example, the magnitude of the stratospheric ozone flux determines whether there is a net production or a net destruction of ozone in the Northern mid-latitude troposphere. The NO_x budgets calculated by the models differ from what is observed by in-situ measurements. This budget is also strongly dependent on transport. To resolve these various discrepancies the contributions of chemical and transport processes have to be analysed. These uncertainties can only be reduced by a coherent programme of global measurements, combining ground based, in-situ and satellite data.

2.4. Radiative Transfer

Radiative transfer in the atmosphere and hence climate forcing are considerably affected by the abundance of trace gases in the UT and in the stratosphere. Although the role of carbon dioxide has been emphasised (and the necessity of understanding the global carbon cycle and its perturbation associated with fossil fuel burning), the climatic role of other radiatively active gases such as water vapour, methane, the CFCs, and ozone has received somewhat less attention.

Water vapour is a rather special case as it is not expected to be the direct cause of changes. However, being the main greenhouse gas, it is expected to govern possible feedbacks in climate changes. This means that it is of fundamental importance to study its distribution and variation throughout the troposphere.

In the stratosphere, the major heating source results from the absorption of solar ultraviolet radiation by ozone. This heating is balanced by cooling produced by infrared emission by CO_2 (15 micron band), ozone (9.6 micron band) and water vapour. In the middle atmosphere, the thermal structure depends on an equilibrium between these radiative processes as well as on heat transport by the general circulation.

In the troposphere, in addition to radiative processes associated with the presence of gases, aerosols, clouds, etc., the temperature profile is affected by latent heat release, convective exchanges, and energy exchange at the surface. The hydrological cycle plays a key role in the thermal processes of this region of the atmosphere.

Climate forcing is not only strongly affected by the abundance of greenhouse gases in the UT/LS but also by the aerosol load and cloudiness. The lack of understanding of the processes which affect the distribution of these radiatively important compounds in this part of the atmosphere has limited our ability to predict future climate changes. For example, it is crucial that continuous measurements of water vapour in the UT/LS be performed, so that not only the direct forcing of water vapour, but also its indirect climate effects (through the formation of clouds) can be better estimated.

It should be noted that the concentration of other radiatively important gases such as ozone is also strongly influenced by the abundance of water vapour, so that a calculation of the ozone concentration in the UT/LS requires that the water vapour abundance be accurately known. Another example is provided by ozone itself. There are almost no reliable data available to verify global chemical transport models that calculate ozone concentration in the UT/LS. Climate predictions must rely on accurate determinations of ozone abundances and their potential future changes as a result of human activities.

Finally, there are interesting and important scientific questions that will have to be investigated in the future that relate radiative forcing (climate) to atmospheric chemistry. For example, the cooling of the LS expected from the increasing abundance of CO_2 and decrease of ozone will probably affect the frequency of occurrence of PSCs, and hence contribute to larger ozone depletion in polar regions. As the level of chlorine will reach its maximum around year 2000–2005, it is possible that the cold temperatures expected in the future will produce a dramatic ozone loss over the Arctic during the winter/spring months (an 'Arctic ozone hole'?). Satellite observations at the turn of the century will be crucial to document such a possible effect.

Another interesting and important question is to assess the climate effect of aircraft effluents in the UT/LS. The release of NO_x by aircraft engines may lead to enhanced ozone concentration in the vicinity of the tropopause, which could affect the climate forcing. A potentially more important effect is the release of water vapour and the subsequent formation of contrails. Not much information exists on the frequency of occurrence of contrails on the global scale, but it is not ruled out that such perturbations could have some impact on radiative forcing in the vicinity of aircraft corridors.

2.5. The Distribution of Chemical Compounds in the Lower Stratosphere and Upper Troposphere

2.5.1. Processes Leading to Enhanced Ozone Loss in the Lower Stratosphere

Global emissions of long-lived chemical species will perturb the levels of active chlorine, bromine and nitrogen compounds, leading to enhanced ozone loss through the reactions discussed above. The species involved include the CFCs, their substitutes and other chlorine containing compounds (e.g. methyl chloroform, CH_3CCl_3), bromine containing compounds (e.g. halons, methyl bromide (CH_3Br)) and nitrous oxide (N_2O).

Enhanced stratospheric particle distribution due to volcanic eruptions will also enhance ozone losses initiated by heterogeneous reactions on the particles as illustrated by the two major volcanic eruptions which have occurred during the last 15 years. Both have significantly perturbed the chemical composition of the LS. The first was the El Chichon eruption in Mexico in 1982 and the second was the Mt. Pinatubo eruption in the Philippines in 1991. Both events pumped large amounts of sulphur and particulate matter into the LS which lead to enhanced stratospheric particle concentrations lasting for two to three years.

Studies have shown that the increases in particle concentrations, coupled with enhanced levels of ozone depleting compounds, lead to significant increases in ozone depletion lasting for periods of up to three years after the eruption. During the next one to two decades, before the levels of chlorine and bromine are expected to decrease (due to reduced emissions of ozone depleting substances), volcanic eruptions which introduce large amount of sulphur into the stratosphere are likely to have a significant impact on ozone levels and the chemical composition of the LS.

The reduction in temperature that has been observed in the LS during the last two decades may also have led to enhanced ozone loss (arising from the resultant increase in PSC formation). Temperatures have been particularly low over the last two years, resulting in extended PSC cloud formation and consequent low levels of ozone in the LS in the Northern Hemisphere (Gathen et al., 1995). However, despite their importance none of these processes is properly (i.e. qualitatively and quantitatively) understood.

2.5.2. Processes Affecting Upper Tropospheric Chemical Composition and Ozone Production

The key chemical compounds for ozone production in the UT are CH_4, CO and NO_x all of which are emitted from pollution sources in the troposphere. Due to their relatively long lifetimes (approximately 9 years for CH_4 and a few months for CO) both CH_4 and CO will be transported from the Earth‘s surface to the UT. CH_4 has been observed to increase throughout the troposphere, while levels of CO have been observed to increase in the Northern Hemisphere, thereby increasing the oxidation process in the troposphere through their reaction with the hydroxyl radical (OH).

Observations have shown that there are large spatial and temporal variations in levels of free tropospheric NO_x and its distribution due to the inhomogeneous distribution of sources and its relatively short lifetime in the atmosphere (only a few days). This leads to large variations in the ozone production and its distribution in the free troposphere, which are very regional in nature.

Two processes involving man’s activities which are of particular relevance to increases in regional levels of upper tropospheric ozone are:

a) NO_x emissions from aircraft – these occur at the level of the tropopause and in the LS, and will therefore depend strongly on stratosphere/troposphere exchange processes. Despite its potential importance little data is available.

b) The regional emission of pollutants (i.e. NO_x, the hydrocarbons and CO) in areas of convective activity – this will normally be sufficiently active to transfer pollutants to the UT where they will contribute to enhanced regional ozone formation (figure 2.7) as well as to radiative forcing (figure 2.8). Observations of the upper tropospheric distribution of compounds like NO_x and CO are essential to gain further insights into the efficiency of the convective processes as well as of their impact on the chemistry of the atmosphere.

The regional character of these processes makes it necessary to study them in regions where air traffic and industrial development are expected to increase over the next two decades (e.g. South East Asia) and to compare them with the unperturbed atmosphere at a global scale.

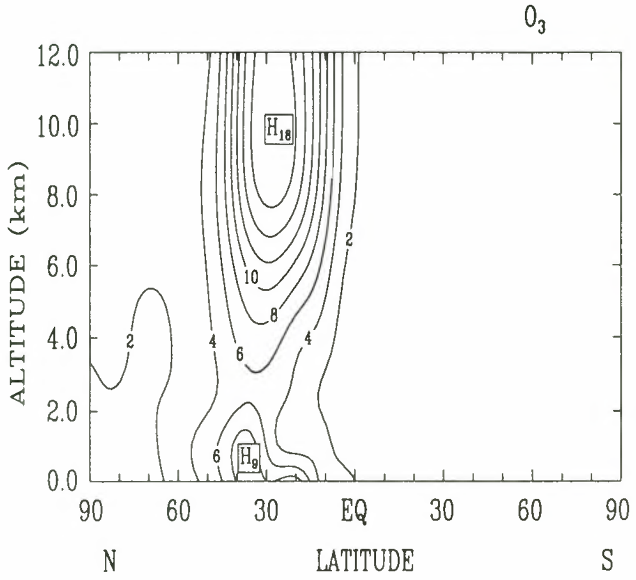


Figure 2.7. Latitudinal/height cross sections of 3-dimensional model calculated increases in ozone levels (in %) between 1980 and 1995 derived from increases in emission of pollutants at the surface. The values are for August (Berntsen et al., 1996).

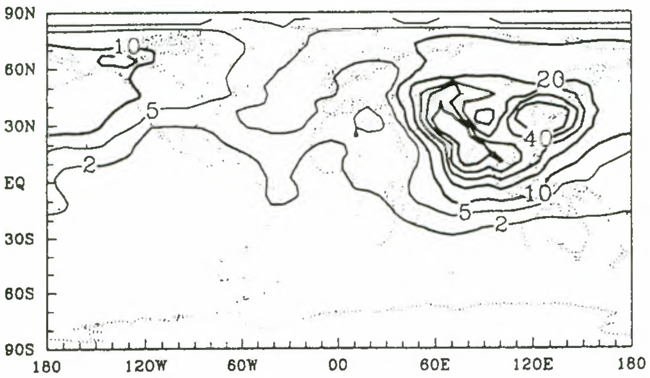


***Figure 2.8.** Calculated increases in the net radiative forcing for the shortwave solar radiation and the longwave radiation (in 10^{-2} W/m^2) for the same increases in ozone. The values are for August (Berntsen et al., 1996).*

2.6. Contribution of Satellite Observations to Atmospheric Chemistry

The climate-chemistry processes discussed in the previous sections have a global dimension that can only be studied with the aid of satellite observations.

2.6.1. Studies by Previous Missions

During the 1990s several spaced-based missions, devoted to the study of atmospheric composition and atmospheric chemistry have been, or will be launched. The UARS mission, launched in 1991, has been followed by further chemistry missions where stratospheric ozone has been measured by several instruments. The latest instrument measuring ozone is the GOME on board ERS-2 satellite which was successfully launched in April 1995. In addition, several missions are presently planned which envisage the provision of specific instruments for chemistry measurements.

These include ILAS and IMG instruments as part of the instrumental payload of the Japanese ADEOS satellite, the microwave radiometer and ultra-violet-visible spectrometer on board the Swedish satellite ODIN (launch 1997), the MOPITT instrument on the US polar platform AM-1, the SAGE III instrument to be launched in June 1998 and the GOMOS, MIPAS and SCIAMACHY instruments on the ESA polar platform ENVISAT (launch in 1999). Around the year 2000 there will be the OMI/GOME and IASI instruments on the ESA/EUMETSAT METOP platform.

These instruments will provide many new insights into stratospheric processes, better ozone measurements and observations of new species.

2.6.2. Contribution by the Proposed Mission

Despite the large numbers of deployed and planned instruments, it is clear that there will only be limited information available on the distribution of key chemical compounds in the LS and UT. Even when available it will not cover the full altitude range or have the spatial (i.e. geographic and vertical) resolution required to properly address the issues discussed above in this highly variable region. The satellite experiment proposed here in this Report (coupled with the contribution of METOP) can help resolve this problem by providing valuable information on the global distribution of these species (including vertical profiles) which will help estimate global budgets and the impacts of man‘s activities, and model the relevant atmospheric processes. In addition, it can complement the ENVISAT mission. None of the current plans properly address the concerns highlighted in this Report.

Areas where the proposed satellite mission should contribute are:

a) In the LS where ozone depletion is affected at mid- to high- latitudes by complex interactions between transport and chemistry.

b) In the UT and at the tropopause where ozone formation could be significant in regions of high emissions from aircraft or in regions to which pollutants are convected from industrialized areas.

c) In areas affected by natural events like volcanic eruptions which perturb the stratospheric composition and the ozone depleting process significantly.

The global significance of such processes can only be properly understood if global observations are provided of key compounds with a geographic and vertical resolution sufficient to characterise regional effects. The selection of the compounds may depend on observation feasibility, but must include the two main actors, namely ozone and water vapour, as well as species that can help in constraining the chemistry and dynamics.

The scientific benefits of atmospheric chemical studies would be strongly increased if field campaigns could be coordinated with satellite observations. Frequent observations in the UT and LS have been made with surfaced-based and airborne instruments through international campaigns. Such activities could further help in the future by providing insights into specific processes and information on local distributions for which satellite observations are less suited.

3. Research Objectives

Drawing on the discussion in the previous chapter the main objectives of the candidate Earth Explorer Atmospheric Chemistry Mission is to significantly advance knowledge and understanding of processes of importance to stratospheric ozone depletion and climate change, with special focus on processes in the UT and the LS. Chemistry, radiation and dynamics are strongly linked in this region through the distribution of ozone.

Of great relevance to the problem of stratospheric ozone depletion are the 1987 Montreal Protocol and later agreements. These are leading to decreases in the anthropogenic release of ozone depleting compounds and are expected to ensure reduced chlorine and bromine levels in the stratosphere. Ozone loss in this region is strongly linked to the emission of chlorine and bromine compounds arising from man made activities. As a result of the international agreement reached through the Montreal Protocol emissions of the major CFCs (CFC-11 and CFC-12) have been steadily decreasing since the latter half of the 1980s. This has resulted in a levelling off in their atmospheric concentrations. It is expected that the chlorine loading of the stratosphere (figure 3.1), which is largely a result of anthropogenic activities, will peak shortly after the turn of the century (WMO, 1995).

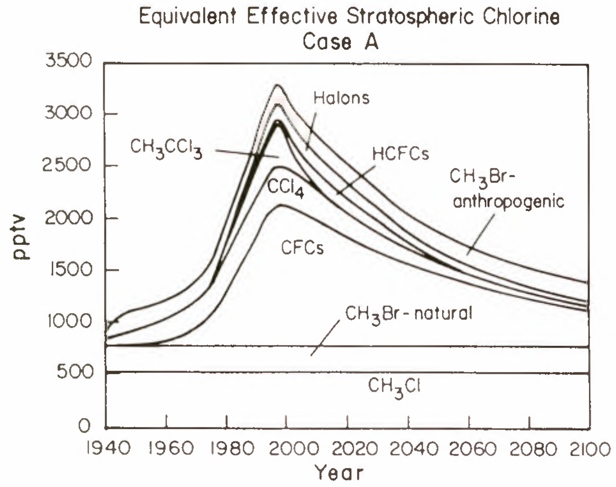


***Figure 3.1**. Estimated equivalent effective chlorine loading in the stratosphere up to present time and in the future. The contribution from the different chlorine and bromine source gases are given. It is expected that the loading will start to decrease around the turn of the century (WMO, 1995).*

It is not clear that the ozone depletion will show a similar behaviour since lower stratospheric ozone depletion at high latitudes, where the largest values are observed, is initiated by the presence of PSCs and the formation of PSCs is very sensitive to changes in the temperatures in the LS. Thus, only a small decrease in the temperatures could lead to a significant enhancement in the formation of PSCs and in ozone loss. Indeed, during the course of the last two to three decades, temperatures in this region of the atmosphere have been observed to decrease by approximately 0.4 K/decade on a global scale at heights of approximately 20 km (pressure levels of 100–50 hPa). This decrease is probably linked to the change in ozone and other greenhouse gases. During the two last winter seasons (1994/1995 and 1995/1996) large ozone losses have been observed at high Northern latitudes which seem to be linked to exceptionally low stratospheric temperatures and the formation of PSCs.

Studies of the radiative impact of ozone and other chemically active gases, together with particles formed by chemical processes in the atmosphere, are an important part of the international assessment of climate change (IPCC, 1995). Chemical and transport processes occurring in the region of the UT and LS are of fundamental importance to chemistry-climate interaction. The lack of global coverage in observations of key compounds, in particular ozone distributions and trends, is a major limitation for assessing the role of ozone as a climate gas.

To address these concerns it is proposed that the Earth Explorer Atmospheric Chemistry Mission should focus on the study of:

The Lower Stratosphere

The main focus here would be on advancing understanding processes of importance for ozone depletion in the height range extending from the troposphere to approximately 30 km. Ozone depletion is of importance for problems related to enhanced UV-B radiation and for the climate-chemistry relation through reduced temperatures.

To this end ozone as well as the species and physical conditions that control its depletion (ClO_x, NO_x, BrO_x, temperature and PSCs) must be measured. Furthermore, HCl should be monitored to assess the effect of the implementation of the Montreal Protocol and SO_2 to correlate changes in ozone chemistry with (possible) volcanic eruptions.

The Upper Troposphere

The main focus here will be the study of the distribution and changes of ozone concentrations in the UT and the key compounds involved in the ozone forming process. This will be of major relevance to the clarification of the role of ozone in climate chemistry interactions.

The distribution of ozone must be properly measured (i.e. good global and regional coverage coupled with quite high vertical resolution). The key compounds in the ozone forming process, notably members of the nitrogen family (including HNO_3), should be measured together with water vapour, methane and carbon monoxide. Observations of them all are important to further understanding of ozone chemistry and the role of transport in the troposphere. In addition observations are required of aerosols and clouds (these affect levels of ultraviolet and visible radiation) and sulphur dioxide which is closely linked to volcanic processes (Figure 3.2).

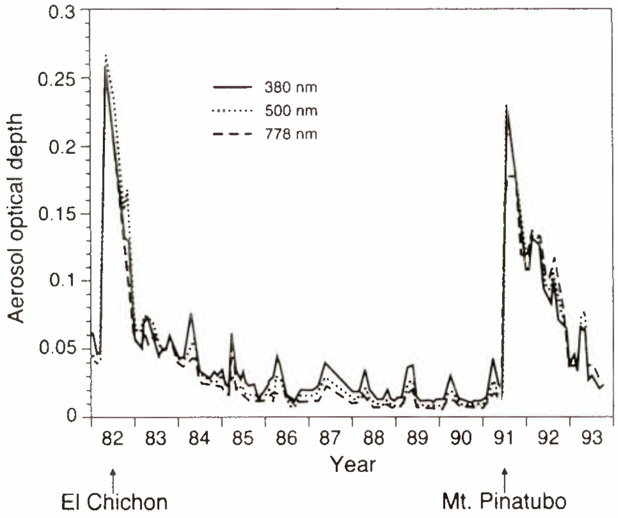


Figure 3.2. *Variation of aerosol optical depth in the stratosphere following the Mt. Pinatubo and El Chichon eruptions (IPCC, 1995).*

Stratospheric/Tropospheric Exchange

The dynamical exchange of chemical compounds through the tropopause and transport of compounds from the lower troposphere to the UT plays an important role in determining the distribution of trace gases and the build-up of compounds in the UT and LS. The transport processes can be modelled provided there is good knowledge of the temperature fields coupled with observations of the distribution of long-lived species such as CH_4, N_2O, SO_2, water vapour and ozone. Transport takes place on different scales so observations at high vertical and geographic resolution are essential.

The observations required to further knowledge and understanding of these three areas will be extremely useful for validating the three-dimensional climate chemistry models which will be used to assess the global environmental effects of chemical emissions and evaluating the corresponding climate changes. At present, and in the foreseeable future, the lack of global data coverage, particularly in UT and LS, of key compounds limits the utility of models for predictions of future climatic changes. Models are now becoming available and there is an urgent need to ensure the provision of the requisite for global data sets.

4. Observational Requirements

4.1. Introduction

The foregoing discussion has highlighted the deficiencies in our understanding of ozone chemistry and chemistry-climate interactions and the need to improve our knowledge of the processes involved notably in the upper tropospheric and lower stratospheric regions. Progress in addressing these objectives depends on the provision of appropriate data and, despite the critical importance of this region to atmospheric chemistry and hence to climate, there is a relative lack of observations in this part of the atmosphere. This reflects the difficulties encountered in observing this region, whether from the ground (obscured by the low troposphere and limited geographic coverage), from aircraft (often difficult to fly high enough and limited geographic coverage) or from space (obscured by the upper stratosphere and technologies necessary to measure some of the key species have not been available in the past).

As it is not possible to exploit any single technique to address a problem that involves the observation of many variables at a global level, the correct approach must be a combination of local observation campaigns, using ground, aircraft and balloon techniques, with remote sensing from space, based on new observation capabilities as well as capitalising on instruments that have already been developed (and in some cases are already scheduled to be launched) and atmospheric models. Observation campaigns can provide comprehensive information in restricted geographic regions, while space observations can provide global observations of key variables.

For remote sensing, observation of the LS/UT region requires the exploitation of spectral regions that:

a) have sufficiently strong spectroscopic features to enable the observation of the target species and at the same time

b) are sufficiently transparent for penetration to low altitudes i.e to the tropopause and below.

Some atmospheric windows in the visible, infrared and millimetre wave regions of the spectrum satisfy these spectroscopic criteria, but only for very few atmospheric species. Generally, stronger spectral features are needed to make nadir sounding observations while better transparency is needed for limb sounding.

Observations from space rely on remote sensing to determine geophysical parameters. Elaborate retrieval processes are required to calculate the geophysical parameters from observed radiances. Therefore, the quality of the data product is directly affected by the sophistication of the ground segment which must, therefore, be considered as an integral part of the mission.

4.2. Geophysical Parameters

The processes that control levels of ozone in the LS and the UT differ markedly (see chapter 2), leading to significant differences in ozone profiles in these two regions. Ideally, a single instrument should be used to determine its height profile with sufficient height resolution to separate changes in the vertical. It is of crucial importance to determine the height regions in which the loss processes lead to reduced levels of ozone and those in which the production processes lead to increases in ozone levels, as changes in the ozone column density determine the impact of UV-B radiation, while changes in the height profile determine the impact of ozone on climate.

A discussion of chemical reactions of particular relevance to ozone depletion in the LS and to ozone generation and climate interaction in the UT, is given in chapter 2. Based on this discussion a list of geophysical variables, which should be measured to adequately address the objectives (chapter 3), have been compiled (see table 4.1). The list includes temperature, important for the characterisation of the physical conditions (and retrievals) as well as aerosols (important for heterogeneous chemistry and climate) and tracers important for studying stratospheric/tropospheric exchange (STE) processes.

For each parameter the table indicates its relevance for the study of the processes occurring in the LS, the UT region and STE (viz. chapter 3).

Ideally, vertical profiles with high vertical resolution (of order of 1 km) coupled with full coverage of latitudinal, longitudinal and seasonal variability are required for each parameter. It is accepted that it would be impossible for the Earth Explorer Atmospheric Chemistry Mission (even if supported by data from other space missions) to meet this very demanding set of requirements. Significant gaps in data provision (whether in the observed geophysical variables or in the spatial coverage of the observations) are still acceptable provided they can occasionally be filled by data from complementary sources (i.e. ground based, balloon borne or air borne) or atmospheric models.

The stratosphere is characterized by stratification of uniform layers and is best studied by limb sounding observations which provide good vertical resolution and poor horizontal resolution. In the troposphere both vertical and horizontal gradients can be present and the three dimensional distribution must be studied. An adequate resolution in three dimensions can be attained by combining limb measurements optimised for vertical resolution with nadir measurements optimized for horizontal resolution. Ideally, the requirement for limb observations is a vertical resolution of 2 km and a horizontal resolution of 500 km in the LS and UT coupled with nadir observations which have a horizontal resolution of 100 km.

Geophysical Variables	**Mission Objective**		
	Lower Stratosphere	**Upper Troposphere**	**Stratosphere Troposphere Exchange**
O_3	*	*	*
ClO_x	*		
NO_x	*	*	*
BrO_x	*		
HO_x	*	*	
CO		*	*
H_2O	*	*	*
CH_4		*	*
N_2O			*
$ClONO_2$	*		
HNO_3	*	*	*
HCl	*		
SO_2	*	*	*
Temperature	*	*	*
Aerosols/PSCs	*	*	
Clouds		*	

***Table 4.1**. List of required geophysical variables*

4.3. Data Sources

In considering the specific data products required to realise the objectives of the Earth Explorer Atmospheric Chemistry Mission (listed in chapter 3), it is logic to distinguish data that should be provided by the Atmospheric Chemistry Explorer itself (i.e. the satellite) from those that might be provided from other sources.

4.3.1. From the Atmospheric Chemistry Explorer

In considering the specific contribution of the Earth Explorer Atmospheric Chemistry Mission to the mission objectives listed in chapter 3 it is important to note at the outset that important new contributions to the study of LS/UT region can be provided by focussing on an instrument operating in the millimetre/sub-millimetre wave region. This reflects its unique properties:

- good transparency in limb sounding geometry,
- reduced effect of scattering by aerosols and clouds,
- possibility to detect some of the key constituents,
- high spectral resolution (can be exploited to attain high vertical resolution),
- continuous observations in emission.

Part of this spectral region has already been used for atmospheric measurements from space (e.g. UARS/MLS), but so far the atmospheric sounding has not been extended to lower altitudes because the observation (spectral) bands used were of insufficient width. Technical advances now make broader observation band widths (with high spectral resolutions) and higher frequencies feasible so this technique is now available for the study of the lower atmosphere. The potential contribution of such an instrument makes it the key element of the proposed Atmospheric Chemistry Explorer.

Geophysical Parameter	**Altitude Range [km]**	**Vertical Resolution [km]**	**Remarks**
O_3	10–25	2	
ClO	15–25	3	
BrO	15–25	5	zonal means
CO	10–20	2	
H_2O	6–25	2	
N_2O	10–25	2	
HNO_3	10–25	2	
HCl	18–25	2	optional
SO_2	10–25	5	special events
Temperature	6–25	2	

Table 4.2. *List of geophysical variables accessible to a limb sounding instrument (mm/sub mm)*

Table 4.2 shows the geophysical variables that could be provided by an Atmospheric Chemistry Explorer based on a mm/sub mm limb sounder. A horizontal resolution of about 500 km should be feasible. It can be seen that many (but not all) of the geophysical variables listed in table 4.1 are included. HCl is included as an option as, although it would be very useful to have available observations of its distribution, these are not considered essential to the realisation of the objectives of the Atmospheric Chemistry Explorer. However, the inclusion of this capability as an option is considered in chapter 6.

Overall such an instrument could provide global, seasonal maps of vertical profile distributions of the observed species. The table does not include all the species/parameters listed in table 4.1 but does include a significant subset of them. The accuracies, resolutions etc. are compatible with the general requirement of a vertical resolution of 2 km and a horizontal resolution of 500 km discussed earlier. The provision and requirements of the other data are considered in the next section.

4.3.2. Complementary Data

The complexity of the data provision required to fully address the scientific objectives of this mission points to the coordinated use of data from other satellites such as METOP and ENVISAT (this is discussed further in chapter 5) as well as from field campaigns that use ground-based, balloon and aircraft measurements. These possibilities are summarised in tables 4.3 (GOME/OMI and IASI on METOP) and 4.4 (MIPAS on ENVISAT). In table 4.3 it should be noted that AVHRR will also play an important role in the provision of cloud observations. This is not specifically indicated in this table. In table 4.4 it should be noted that a vertical resolution of 3 km should be attained with MIPAS.

It will be noted that neither GOMOS nor SCIAMACHY are included in table 4.3, the former because its geographic and species coverage is incompatible with the other elements of the Earth Explorer Atmospheric Chemistry Mission, the latter because of the relatively small incremental return of SCIAMACHY data, over the GOME/OMI/IASI combination on board of the 'simultaneous' METOP series of satellites, seen within the context of this mission.

It can be seen that important contributions of METOP data to this mission include nadir sounding (with high spatial resolution) of some key species as well as information on cloud coverage and aerosol concentration.

Assuming an overlap (in time) between the ENVISAT and the Atmospheric Chemistry Explorer, then the MIPAS instrument could provide complementary measurements of active species of the nitrogen family, of the reservoir species $ClONO_2$ (important for the chlorine budget) and of stable compounds suitable for studies of stratospheric/tropospheric exchange. As MIPAS could contribute significantly to the mission it is also considered as an option in chapter 6. The optional addition of SCIAMACHY is not included in chapter 6 as the 'delta' of its contribution is considered difficult to justify within the context of the Earth Explorer

Atmospheric Chemistry Mission assuming that both GOME/OMI and IASI fly on METOP. But certainly the advantage should be taken of the SCIAMACHY data to further strengthen the Earth Explorer Atmospheric Chemistry Mission.

Geophysical Variable	**GOME/OMI**	**IASI**	**Remarks**
O_3	Profile (5 km res.)	Column	
ClO	Column		Ozone hole
OClO	Column		Special events
NO_2	Column		
BrO	Column		Zonal Means
CO		Column	
H_2O	Column	Profile (1 km res.)	
CH_4		Column	
N_2O		Column	
SO_2	Column		Special events
Temperature		Profile (1 km res.)	
Aerosols/PSCs	Column		
Clouds	Detected	Detected	

Table 4.3. *The potential contribution of nadir viewing GOME/OMI and IASI instruments on METOP (AVHRR is not included)*

Some species not included in table 4.1 are included in tables 4.3 and 4.4 but conversely not all the species listed in table 4.1 appear in the other two tables. This leads to the requirement for complementary measurement campaigns.

The main objectives of these campaigns should be twofold, namely the validation (with high spatial resolution) of the space observations and the provision of complementary measurements on e.g. the HO_x chemistry in both the troposphere and the stratosphere (it is assumed that observations of HO_x would be difficult from space) and on NO_x chemistry in the troposphere.

Geophysical Variable	**Altitude Range* [km]**
O_3	12–80
CFCs	5–20
NO_2	15–46
NO	20–60
N_2O_5	22–28
CO	20–60
H_2O	7–85
CH_4	5–65
N_2O	5–48
$ClONO_2$	19–25
HNO_3	10–37
Temperature	stratosphere

* 20% accuracy limits.

Table 4.4. *The potential contribution of MIPAS*

4.4. General Characteristics of the Atmospheric Chemistry Mission

It follows from the preceding discussion that the orbit and the timing of the Atmospheric Chemistry Mission must be chosen in such a way as to make best use of the complementary measurements provided by other missions and the ground segment. It should have an orbit synchronized with that of METOP, and be early enough to have an overlap with the MIPAS and SCIAMACHY measurements on ENVISAT. Since both are a particularly important complement to the Atmospheric Chemistry Mission, the overlap between them should be as long as possible, in any case not less than one year. The overall duration of the Atmospheric Chemistry Mission should ideally be of the order of four years with a minimum of two years. Furthermore, the mission must be implemented in such a way as to allow the assimilation of data from different sources.

The requirement for global observations implies the use of a polar sun-synchronous orbit. Sampling requirements are driven by the requirement of (near) simultaneous observations of the same air sample with both nadir sounding (i.e. OMI/GOME and IASI on board METOP) and limb sounding instruments (on board the Atmospheric Chemistry Mission and MIPAS/ SCIAMACHY on ENVISAT).

Given the relatively long time constant of most atmospheric processes, it is argued that measurements can be considered to be concurrent (i.e. simultaneous) when taken with a time difference of less than 5 minutes. Limb sounding observations must have a horizontal resolution of 500 km and its optical path in the atmosphere (at altitudes between 8 and 25 km) must be contained within the swath of the nadir sounding observation. Overlap between observations of Atmospheric Chemistry Mission and METOP must be maintained throughout the mission with knowledge of the relative geographical locations of nadir and limb observations better than 50 km. Given their horizontal weighting function, two limb sounding measurements can be considered to observe the same air sample when their optical paths have a distance smaller than 200 km at the relevant atmospheric altitudes.

4.5. Fulfilment of Research Objectives

The discussion of observational requirements and the way it is proposed to address them is summarised in Table 4.5. This lists the target species and geophysical parameters and the potential contribution(s) of the various mission components (space observations only). In each case it should be borne in mind that there is (ideally) a requirement for observations with a vertical resolution of 2 km and an horizontal resolution of 500 km in the LS and UT coupled with (nadir) observations which have a horizontal resolution of 100 km. It also summarises the potential contribution of SCIAMACHY.

Target Variable	Actual Variable Observed	Atmospheric Chemistry Explorer	METOP GOME /OMI	METOP IASI	ENVISAT MIPAS[2]	ENVISAT SCIAMACHY[5]
O_3	O_3	10–25 km	Profile	Column	12–80 km	Contribution
ClO_x	ClO	15–25 km	Column	–	–	Contribution
	OClO	–	Column[3]	–	–	Contribution
	CFCs	–	–	–	5–20 km	–
NO_x	NO_2	–	Column	–	15–46 km	Contribution
	NO	–	–	–	20–60 km	Contribution
	N_2O_5	–	–	–	22–28 km	–
BrO_x	BrO	15–25 km[6]	Column	–	–	Contribution
HO_x[1]	–	–	–	–	–	–
CO	CO	12–18 km	–	Column	20–60 km	Contribution
H_2O	H_2O	6–25 km	Column	Profile	7–85 km	Contribution
CH_4	CH_4	–	–	Column	5–65 km	Contribution
N_2O	N_2O	10–25 km	–	Column	5–48 km	Contribution
$ClONO_2$	$ClONO_2$	–	–	–	19–25 km	–
HNO_3	HNO_3	10–25 km	–	–	10–37 km	–
HCl	HCl	18–25 km[3]	–	–	–	–
SO_2	SO_2	10–25 km[7]	Column	–	–	Contribution
T	T	6–25 km	–	0–25 km	–	Contribution
Aerosols /PSCs	Aerosols /PSCs		some data		some data	some data
Clouds[4]	Clouds		some data	some data	some data	some data

Notes:

1. It assumed that HO_x can be derived from calculations validated by measurement campaigns.
2. 20% accuracy limits.
3. Optional measurement on the Earth Explorer Chemistry Mission.
4. Excludes the contribution of AVHRR
5. SCIAMACHY can view in both limb and nadir
6. Zonal means
7. Special events

Table 4.5*. The potential contributions to the Earth Explorer Atmospheric Chemistry Mission*

5. Mission Elements

5.1. Space Segment

Taking account of the observation requirements listed in chapter 4 and the likely capabilities of space-based instruments in the year 2000, table 5.1 links observation requirements to potential data sources. It should be noted that different instruments provide complementary data not only in their coverage of the geophysical variables but also in altitude coverage and vertical resolution.

Geophysical variable	**On ACE**	**On METOP**	**On ENVISAT**	**Other**
Ozone	MASTER	OMI/GOME, IASI	MIPAS, SCIAMACHY	
Temperature	MASTER	IASI	MIPAS, SCIAMACHY	
ClOx	MASTER	OMI		
NOx			MIPAS, SCIAMACHY	Airborne
BrOx	MASTER	OMI/GOME		
HOx				Airborne
CO	MASTER	IASI	MIPAS, SCIAMACHY	
H_2O	MASTER	IASI, OMI/GOME	MIPAS, SCIAMACHY	
CH_4		IASI	MIPAS, SCIAMACHY	
N_2O	MASTER	IASI	MIPAS, SCIAMACHY	
$ClONO_2$			MIPAS	
HNO_3	MASTER		MIPAS	
HCl	MASTER (option)			Ground/ Airborne
SO_2		OMI/GOME	SCIAMACHY	
Aerosols/PSCs		OMI/GOME	SCIAMACHY	
Clouds		AVHRR, OMI/ GOME, IASI	SCIAMACHY	

Table 5.1. *Data sources for the Earth Explorer Atmospheric Chemistry Mission*

The proposed baseline for the Earth Explorer Atmospheric Chemistry Mission will consist of:

- A dedicated Atmospheric Chemistry Explorer satellite (ACE) carrying MASTER (Mm-wave Acquisitions for Stratosphere/Troposphere Exchange Research) and GRAS (GPS/GNSS Radio Occultation Atmospheric Sounder) as described in chapter 6.

- The utilisation of the chemistry observations of the METOP satellite (i.e. of OMI/GOME and IASI) in addition to the utilisation of AVHRR for cloud coverage detection.

- The utilisation of information on NO_x derived from the MIPAS observations obtained during the first half of the ENVISAT mission. The coincidence in orbit of ACE with ENVISAT (MIPAS and SCIAMACHY) during the second half of the ENVISAT mission would further enhance the results of this Explorer mission.

The characteristics of the relevant chemistry observing ENVISAT and METOP instruments are assumed to be as follows:

Ozone Monitoring Instrument (OMI)

It is proposed that OMI should be based on GOME type instrument currently flying on ERS-2. GOME is a nadir looking, across-track scanning spectrometer with +/- 30 deg swath (equivalent to 960 km at METOP altitude). It is intended to observe:

- profiles of O_3;
- column contents of NO_2, HCHO, NO, H_2O, SO_2, ClO, BrO, OClO, O_3, O_2;
- aerosols and PSCs.

It observes in 4 bands which have the spectral resolution widths shown below.

240-295 nm	290-405 nm	400-605 nm	590-790 nm
0.11 nm	0.12 nm	0.2 nm	0.2 nm

GOME also provides polarization detection, which is expected to be improved for OMI, thus enhancing its capability for aerosol detection.

Infrared Atmospheric Sounding Interferometer (IASI)

IASI is a nadir looking, Fourier-transform sounder with the following measurement objectives of relevance to the Earth Explorer Atmospheric Chemistry Mission:

- temperature profiles in free troposphere and LS with 1 K accuracy and 1 km vertical resolution;
- water vapour profiles with 10% accuracy and 1 km vertical resolution;
- column contents of O_3, CO, CH_4, N_2O with target accuracies of 10% (5% for O_3)

It operates in 3 bands: 8.26-15.5 μm, 5-8.26 μm and 3.4-5 μm.

IASI has a built-in 64 x 64 pixel imager with 700 m resolution centred in the line of sight of the scanner. The imager includes a 3.7-4.0 μm channel for cloud detection.

Michelson Interferometer for Passive Atmospheric Sounding (MIPAS)

MIPAS will view in the limb, measuring the concentration profiles of atmospheric constituents on a global scale. It will observe atmospheric limb emissions throughout the mid-infrared region, allowing (amongst other parameters) it to detect the complete family of NO_x compounds as well as the CFCs.

It operates in the mid-infrared spectral region from 4.15 to 14.6 μm and providing data about the concentration profiles, it will also provide insights into latitudinal variations and horizontal gradients for the species of interest. Further information on MIPAS is given in section 6.7.

In general terms, SCIAMACHY is an instrument similar to GOME/OMI, with additional channels at 790-1055 nm, 1000-1700 nm, 1940-2040 nm and 2265-2380 nm. It is capable of viewing in limb as well as in nadir.

5.2. Ground Segment

Conceptually the ACE satellite ground segment consists of four elements:

- a command and data acquisition station;
- a mission operations and satellite control element;
- a processing and archiving element;
- a science data centre.

The Processing and Archiving Element would process the ACE data to Level 1b before being transferred to the Science Data Centre which would produce the Level 2 products. It would also provide archiving facilities. The ACE data are then assumed to be transferred to a science data centre which would merge data from ACE, METOP, ENVISAT, etc.

6. System Concept

6.1. General

The baseline Earth Explorer Atmospheric Chemistry Mission concept is schematically shown in figure 6.1. The space segment includes a new satellite, the Atmospheric Chemistry Explorer (ACE) carrying as its main instrument MASTER with GRAS as a passenger. The mission is intended to exploit synergistically the observations provided by ACE (MASTER), METOP (OMI, IASI) and ENVISAT (MIPAS, SCIAMACHY).

This approach of symbiotically using the observations from 3 satellites allows the implementation of the additional new observations on a small platform making it possible to propose a very cost effective Earth Explorer Atmospheric Chemistry Mission. The combination of measurements taken from ACE (limb) and METOP (nadir) is optimum as the two different types of measurement geometries can only be properly synchronised when the two different classes of instrument are on two different satellites.

The synergy (i.e. the overlap for the first part of the ACE mission) ACE-ENVISAT allows the consolidation of understanding the NO_x chemistry derived from the first years of operation of ENVISAT. This could be achieved by planning MIPAS observations from ENVISAT to be periodically coincident with MASTER observations from ACE.

6.2. ACE Payload

6.2.1. MASTER

Objectives

MASTER (Millimetre-wave Acquisitions for Stratosphere/Troposphere Exchange Research) is a passive spectro-radiometer operating in the millimetre-wave spectral region, measuring globally and continuously, the self-emission of the atmosphere in a limb sounding geometry.

The target species are:

H_2O, CO, ClO, O_3, HNO_3, SO_2, N_2O, H_2O_2, CH_3Cl, BrO

To get essential information on atmospheric pressure and temperature required for retrievals, the spectral signature of O_2 is also observed. The objective of MASTER is to deliver calibrated spectra of the atmosphere as a function of limb view.

Instrument Requirements

The most important instrument requirements are listed in table 6.1.

Azimuth pointing	3 directions	–10, 0 , 10 deg
Elevation height	Range	–5 to 150 km
	Accuracy	1 km
	Knowledge	0.2 km (bias excluded)
	Stability	0.2 km
Beam efficiency over tangent interval	Band A	85% over 4.5 km
		98% over 9 km
	Bands B, C, D	85% over 3 km
		98% over 6 km
	Band E	85% over 2 km
		98% over 4 km,
Nominal elevation scan	Scanning speed	0.3 s/km
	Main portion of scan	0 to 25 km
	Occasional extension	25 to 50 km
Spectral range	Band A	199.0 to 207.0 GHz
	Band B	296.0 to 306.0 GHz
	Band C	318.0 to 326.0 GHz
	Band D	342.0 to 348.0 GHz
	Band E	498.5 to 505.0 GHz
Spectral resolution	50 MHz over all spectral range	
	3 MHz over two 600 MHz wide channels	
Spectral accuracy	0.05 MHz	
Noise equivalent temperature @ 50 MHz resolution, 0.3 s integration	Band A	1.0 K
	Bands B, C, D, E	1.5 K
Radiometric accuracy	Absolute	1 K
	Relative	0.1 K
Sideband rejection	30 dB	

***Table 6.1**. Main MASTER requirements*

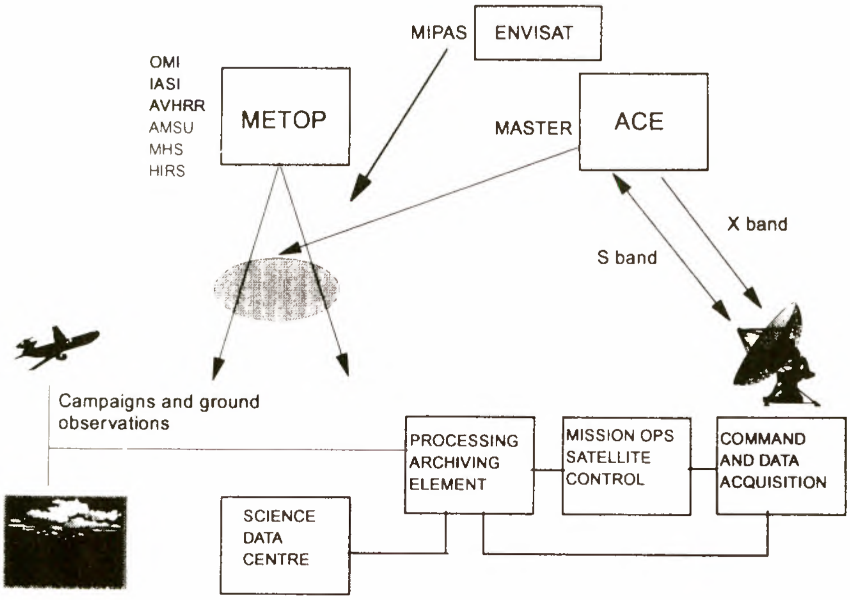


Figure 6.1. Overview of the Earth Explorer Atmospheric Chemistry Mission

Operating principle and overall system concept

Two instrument concepts, referred to hereafter as A and B, have been studied at pre-phase A level. The architecture and the operation principle underlying both concepts are similar. They are described below and illustrated in figure 6.2.

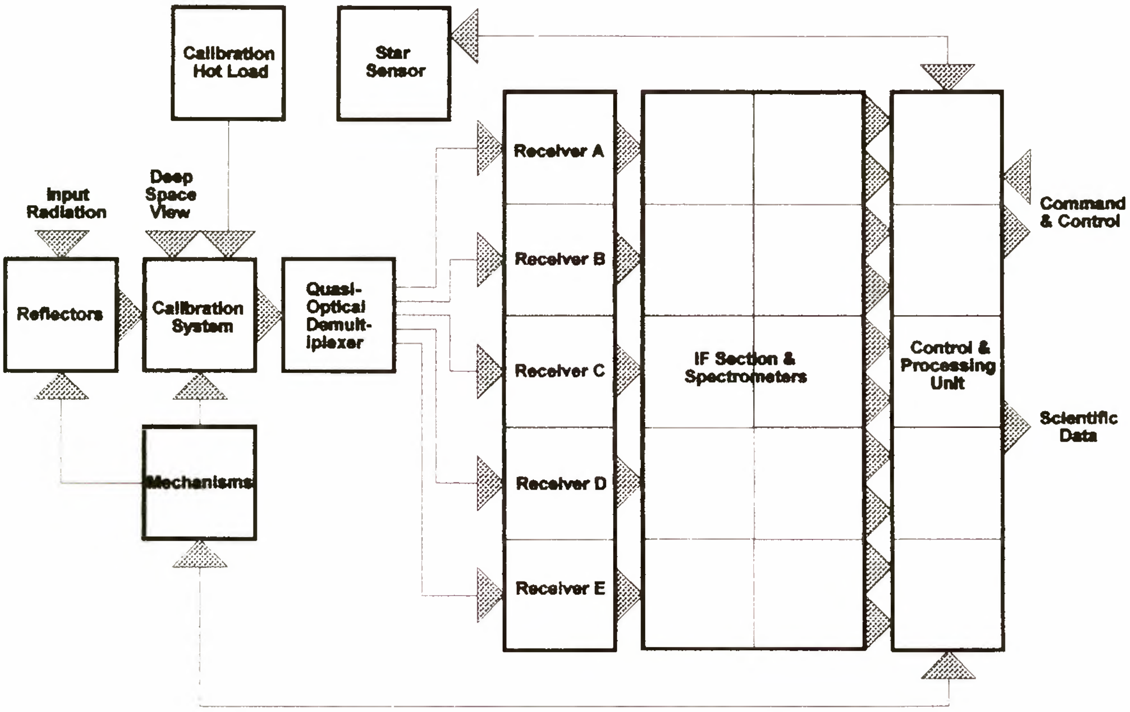


Figure 6.2. MASTER functional architecture and operating principle

Even from a low Earth orbit, the limb sounding geometry imposes a requirement of extremely high directivity on observations. To ensure that a single spectrum is representative of the emission of an atmospheric limb not thicker than a few kilometres, MASTER requires a 2 metre long antenna (very similar to an all-reflective optical telescope). Through passive filtering surfaces, the signal gathered by the antenna is separated in a quasi-optical demultiplexer into 5 different frequency regions, which are sent in parallel to the receiver subsystem.

Detection is performed with 5 heterodyne receivers with receiver input signals being combined with continuously produced local oscillator signals of approximately the same frequencies (or submultiples) as the input signals. Such an element, called the mixer, performs a down-conversion of the original signal to a lower frequency, while preserving amplitude and phase information. Output signals, much lower in frequency by typically a factor 10 or more, are then amplified and further processed.

In the spectrometer subsystem, the amplitudes of the different frequency components of the output signals from the receivers are measured, such that spectra can be fabricated.

To generate the required spectra as a function of altitude, MASTER sequentially performs measurements by integrating spectrally analysed signals over 0.3 second intervals, smoothly moving the antenna at a constant rate of 0.3 second per (tangent height) kilometre at the limb. After a few such elevation scans, lasting typically 10 seconds, the responsivity of MASTER is characterised by performing a measurement of deep space and a measurement of a calibrated hot load.

Figures 6.3 and 6.4 show possible configurations.

For both concepts, the antenna subsystem, the quasi-optics and the receivers are in close proximity, while the intermediate frequency (IF) section, the spectrometers and the control unit are packaged in a separate unit. This separate box can be handled similarly to the other satellite electronic boxes, and can be either installed on a different face of the platform or accommodated inside the spacecraft.

The obvious outstanding feature of MASTER is the long primary reflector, which is 2 m in length. The antenna benefits from the practical absence of requirements on beam efficiency along the azimuth direction, which means that the reflector does not need to be circular. The shape is thus elliptical, with an axial ratio of about 2:1.

Concept A assumes room temperature operation. Concept B uses passive cooling to achieve a receiver temperature of about 200 K. Lowering the operating temperature has the effect of increasing sensitivity by a small factor. It is advisable to further trade-off cooling, complexity and sensitivity.

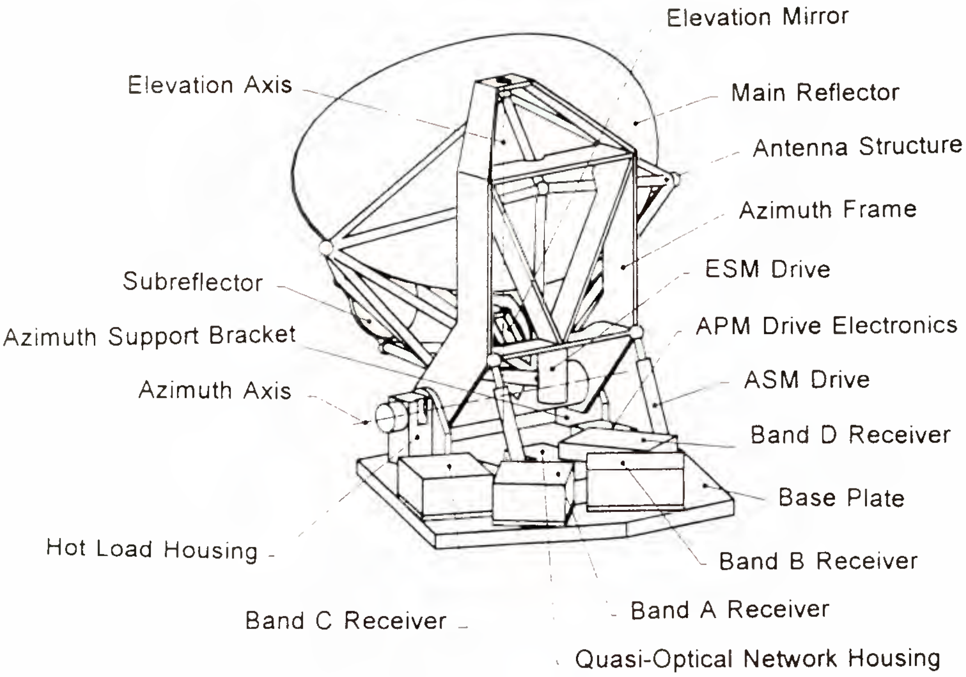


***Figure 6.3**. MASTER: configuration Concept A*

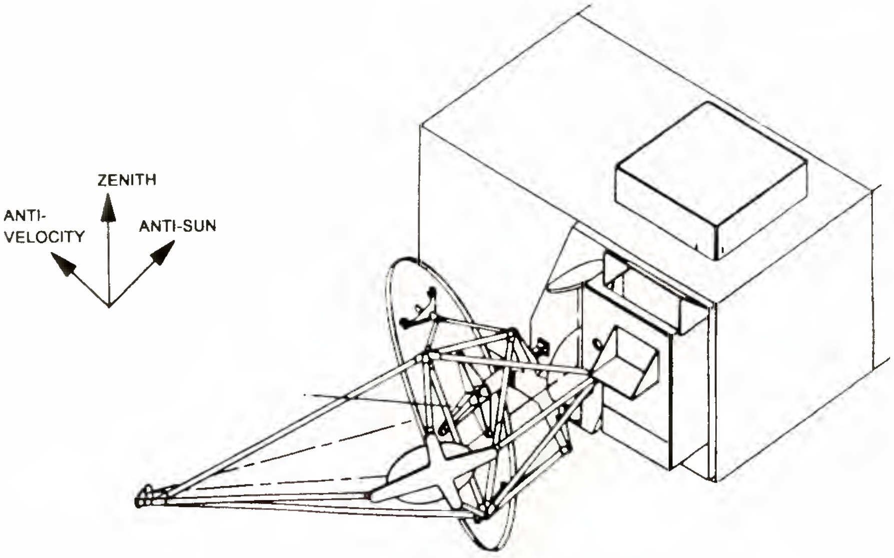


***Figure 6.4**. MASTER: configuration Concept B*

Subsystem concepts

The following section provides a summary description of the main subsystems which have a direct impact on performance. Ancillary equipment has been omitted for simplicity.

- *Antenna and mechanisms*

Vertically, the primary reflector has a length of approximately 2 metres, imposed by the requirement for high spatial resolution at the limb in the elevation direction. Horizontally, its length is smaller (about 1 metre.)

The main function of the antenna is to relay the desired limb emitted radiation to the quasi-optics. To do this, both concepts use a single beam approach and mechanical scanning. However the electrical configuration and the scanning method differ significantly.

Concepts A and B both use subreflectors located respectively before and after the focus of the primary reflector. Concept A is more compact, which is attractive for accommodation.

For both concepts, azimuth pointing (if not provided by the platform) is achieved by rotating the primary reflector and the subreflector together. For the elevation scan, which takes place only over a few degrees, Concept A moves both reflectors, but Concept B rotates only the primary reflector.

Locking devices are required to withstand the launch vibrations. However, deployment as such is not necessary and should be avoided, since tolerances on relative positions of antenna reflectors are tight.

Both concepts propose CFRP as primary reflector material. The surface accuracy of the primary reflector should be in the 5 to 10 μm range. This is challenging and effects such as thermal distortions, outgassing and zero gravity will have to be investigated in detail. Testing of the antenna will also need further assessment.

Concept A uses a 'conventional' hot load design with pyramidally structured cavity walls, while Concept B is based on absorbing surfaces giving specular reflections.

Including structure, mirrors leading to the quasi-optics (including switching mirror), the hot load, the single axis star-sensor (to satisfy the strict elevation pointing and pointing knowledge requirements), for both concepts the antenna subsystem would consume about 25 W and weigh approximately 75 kg.

- *Quasi-optics and receivers*

The quasi-optics and receivers concepts can be separated in the following assemblies:

- demultiplexing circuitry
- sideband filters
- local oscillator injection circuitry
- mixer
- local oscillator
- first intermediate frequency amplifier

The sideband filtering and local oscillator injection assemblies differ significantly for the two concepts. Since Concept A uses fundamentally pumped mixers, local oscillator injection is necessary in the quasi-optics. It is assumed that a single beamsplitter plate will allow signal transmission, sideband reflection and local oscillator reflection. This plate has to be developed. Concept B uses subharmonically pumped mixers so local oscillator injection is then not carried out in the quasi-optics. Four beamsplitters are nevertheless used in this design, two of them necessary for harmonic rejection, and two others for sufficient sideband rejection. This design is rather conservative.

The mixers of Concept A consist of waveguide mounted whisker contacted Schottky diodes with corrugated horns being used as feeds. The mixers operate at room temperature. The phase locked local oscillator signals are generated from Gunn diodes, followed by multipliers. The IF range is from 20 to 30 GHz. Completely redundant receiving chains have been assumed. First IF amplifiers are based on high electron mobility transistors (HEMTs).

Concept B uses waveguide mounted planar Schottky diodes for its mixers and corrugated horns as feeds. The mixers and first intermediate frequency amplifier are cooled passively to 200 K. Local oscillator signals, at about half the signal frequency, are injected using waveguides. Gunn diodes are used to generate these signals. Multipliers are necessary for bands B to E. The IF range is from 5.5 to 18.5 GHz. Redundant mixers have been selected with switching mirrors, and redundant local oscillators with waveguide switches. The first IF amplifiers are also based on HEMTs. Band B (widest with 10 GHz) is separated in 3 subbands and thus uses 3 amplifiers for better sensitivity.

The quasi-optics and receivers would have a mass of about 125 kg and would consume about 125 W of power.

- *Spectrometers*

As the receiver bands are wider than can be accommodated by individual spectrometer units, both concepts need an IF section to subdivide the bands into smaller channels.

Concept A uses acousto-optical spectrometers. Each spectrometer unit covers 10 GHz and consists in fact of 5 units, each covering 2 GHz, sharing the same acousto-optical cell. For band E, 4 units would be sufficient. Development of the 2 GHz cell is on-going (current achievement is 1.5 GHz). Development of the five-fold package is further required. As these spectrometers intrinsically deliver high resolution information (< 3 MHz), they are used for both 50 MHz and 3 MHz resolution requirements.

Concept B uses digital auto-correlation spectrometers. The individual low resolution units have a bandwidth of 1.25 GHz. The two high resolution units each have a bandwidth of 600 MHz. Development of this technology is required.

The mass of both concepts would be about 35 kg. Power consumption for Concept A would be about 125 W, while for Concept B it should be about 250 W. Redundancy is implemented in both concepts by providing extra spectrometer units.

Status of conceptual design performance

Both concepts already meet or nearly meet the requirements. The issues described below are typical of any space instrument development at the present stage of definition.

For Concept A, compliance with spectral accuracy has been claimed. However it is still to be demonstrated that the centre frequency of all spectrometer spectral elements (3 MHz width) can be characterised easily with an accuracy better than 100 kHz. For Concept B, the accuracy is ensured by the design.

Both concepts are nearly compliant with noise equivalent temperature requirements. Although compliance with radiometric accuracy is marginal, in particular with relative radiometric accuracy, the requirements have to be optimised by further study of their implications in scientific terms.

The total predicted mass and power consumption are: Concept A: 320 kg, 350 W. Concept B: 290 kg, 470 W. However, power estimates in particular are highly dependent upon the outcome of new spectrometer developments. 350 kg and 400 W have been used in section 6.4 and 6.7 as inputs to the overall satellite mass and power budgets.

Both concepts require redundancy for mixers, local oscillators and spectrometers, to approach a 90% reliability figure for a 5 year mission duration.

Key technologies

The high surface accuracy requirements on the primary reflector represent a major technical challenge. State-of-the-art manufacturability and effects like zerogravity, thermal gradients and launch conditions will have to be assessed.

In receivers and quasi-optics, development work is required for the mixers, but the technologies are in principle proven. Image band rejection for concept A is based on the use of a single beamsplitter, a component which has to be developed. A fall back position has been identified which, however, requires more components.

For both concepts, spectrometers require significant developments. Different spectrometer types are however interchangeable without significantly affecting the front ends. The development effort can be further traded off against mainly higher power consumption.

6.2.2. GRAS

It is proposed that a GPS/GNSS receiver will be used for position determination and for provision of the time reference on-board ACE. However, if a receiver like GRAS is embarked, it can also perform atmospheric sounding in both the stratosphere and UT.

GRAS is the GNSS Receiver for Atmospheric Sounding that is being developed in anticipation of the Earth Explorer Gravity Field and Steady-State Ocean Circulation (ESA, 1996a) and the Earth Explorer Atmospheric Profiling (ESA, 1996b) Missions. The performances currently expected for the atmospheric sounding function are based on simulation studies and on the exploitation of flight data from the GPS-Met experiment.

Temperature	better than 1 K at vertical resolutions of 0.5–1 km in LS and UT degrading to 2 K at 50 km altitude
Water vapour	10% in planetary boundary layer throughout mid latitudes and tropics and at mid latitudes in the mid troposphere at pressures greater than about 600 hPa

Details of the GRAS sounding mission and of the instrument itself can be found in the Report for Assessment of the Earth Explorer Atmospheric Profiling Mission. GRAS will have a mass of 6 kg and require 15 W of power. It will generate 10 kbps of data on average corresponding to 1100 sounding profiles/day.

It is proposed that GRAS will be on METOP and on ACE. The ACE-METOP tandem offers pairs of occultation events with relatively small spatial and temporal separation. This configuration is very attractive as it allows the investigation of cases of unfavourable horizontal variability.

6.3. Mission and Operations Profile

The orbit of ACE must be selected to exploit the synergy with the METOP instruments. MASTER would sound in the limb the volume of atmosphere being observed at nadir by the METOP instruments. This implies the selection for ACE of the same orbit as METOP, i.e. sun-synchronous, 820 km altitude, 09:30 local time of descending node. ACE has to be ahead of METOP as shown in figure 6.5.

No orbit maintenance requirements are imposed by this mission on METOP. For ACE the orbit maintenance strategy is designed to guarantee that the time difference between the observation of a given part of the atmosphere by MASTER on one side and IASI and OMI/GOME on the other side is less than the difference inherent to limb and nadir sounding instruments if they were located on the same platform, i.e. around +/- 7 minutes equivalent to around 2800 km of distance along the subsatellite track. The tandem ACE-METOP improves the observation conditions by reducing this difference.

The strategy will consist of maintaining ACE around a nominal position located 27.7 deg ahead of METOP on the same orbit. In fact ACE will describe a 'boomerang' trajectory with respect to this nominal position, from a location above and ahead, crossing the METOP orbit behind this nominal position and going below and ahead until a maintenance manoeuvre is required as shown in figure 6.6.

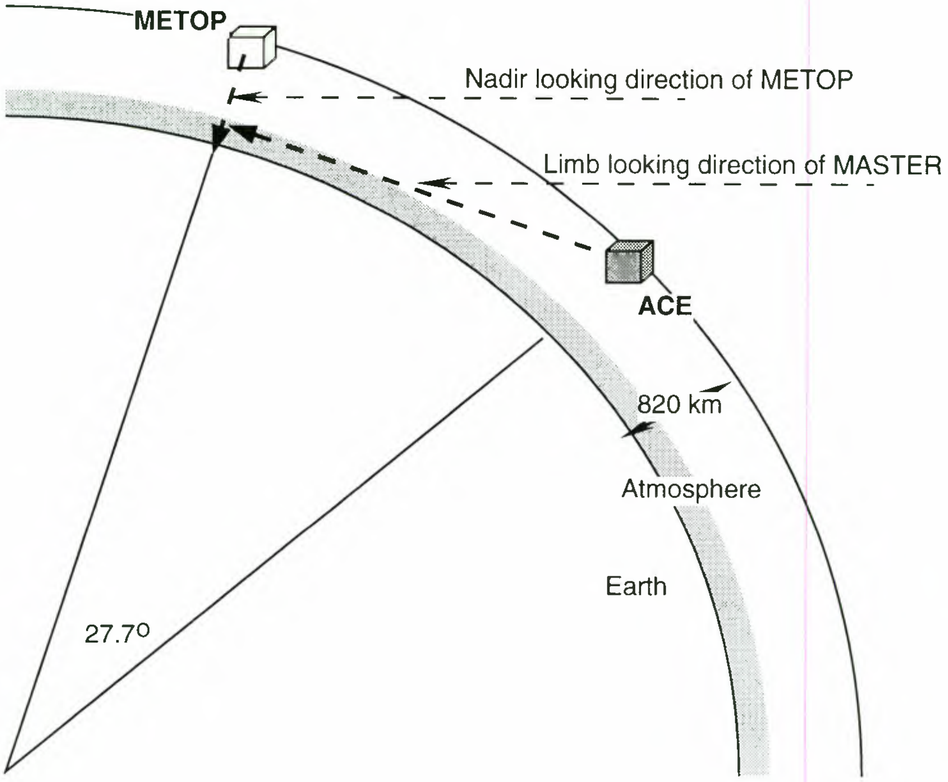


Figure 6.5. Observation geometry for the Earth Explorer Atmospheric Chemistry Mission

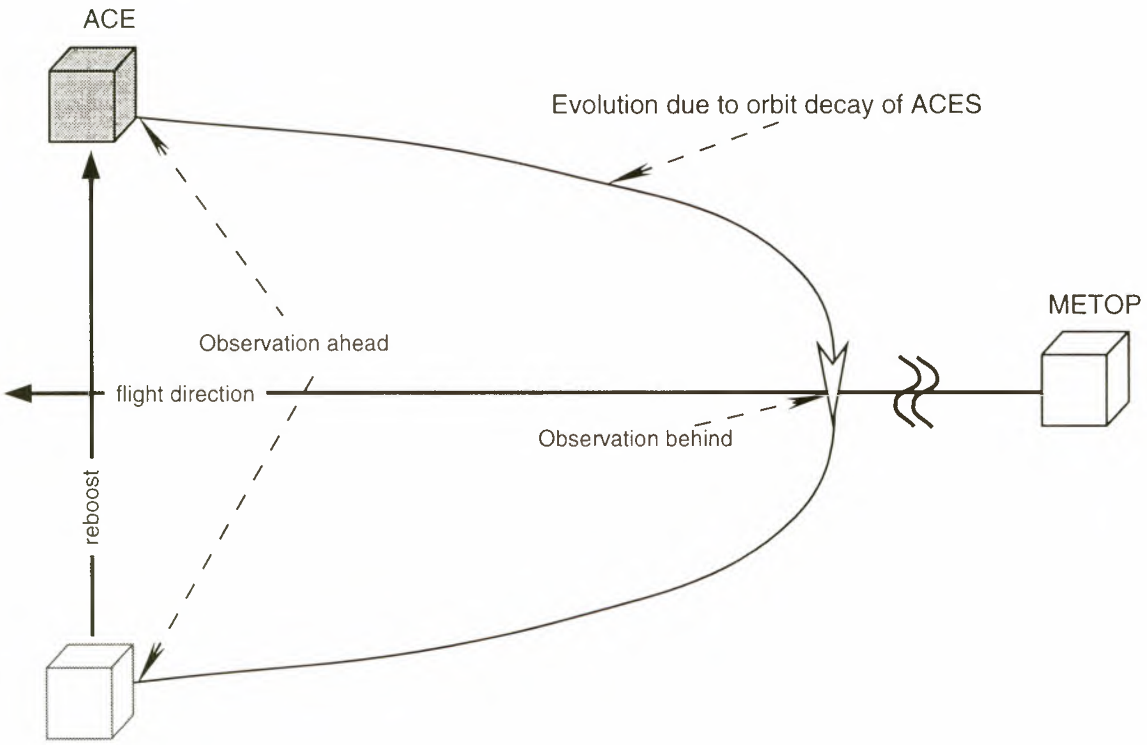


Figure 6.6. *ACE orbit maintenance strategy: ACE would be placed ahead and above METOP. Due to the natural orbit decay it would approach the nominal METOP orbit and advance it again. A reboost manoeuvre would put it back to the initial position and the cycle repeats.*

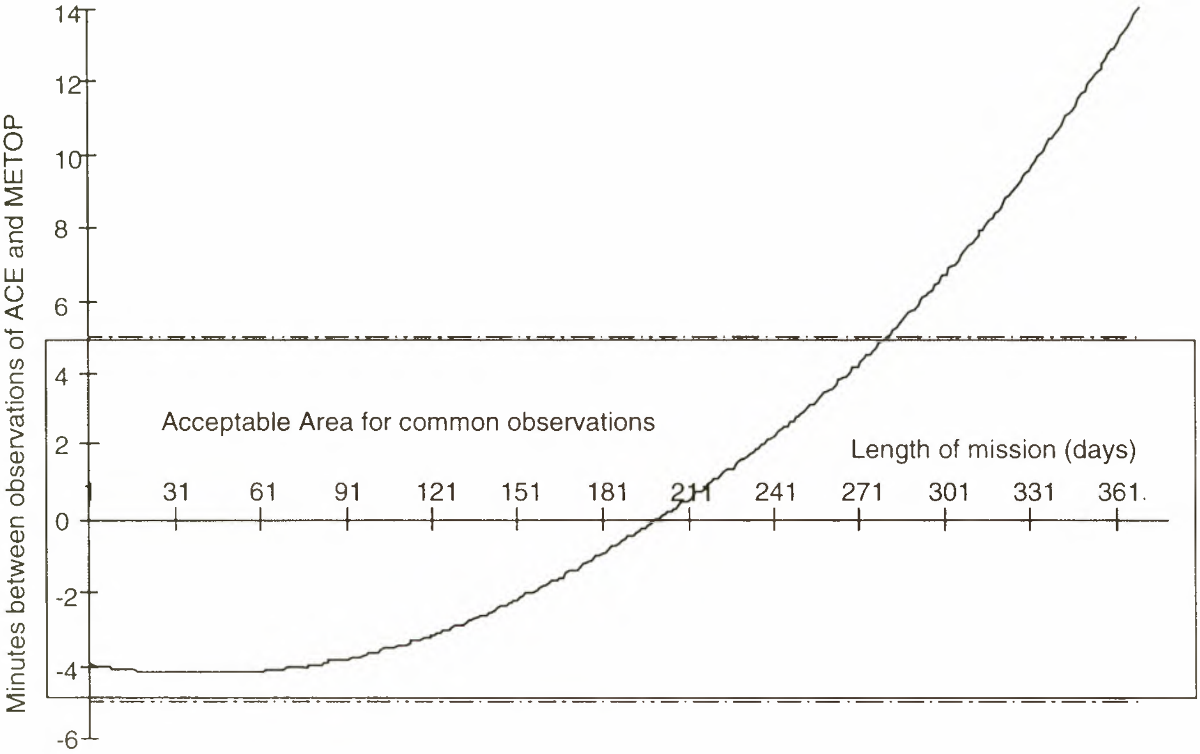


Figure 6.7. *Evolution of the ACE - METOP observation geometry*

Assuming the METOP orbit is maintained and the ACE orbit left to decay, preliminary calculations show that it would take at least 9 months before the observations would be time-separated by more than 5 mins (see figure 6.7) i.e. orbit maintenance would be very infrequent.

At this altitude, the effect of drag on ACE is very small and for mean solar activity the orbit decay can be estimated to be about 0.1 m / orbit. The total delta V for altitude maintenance is around 5 m/s for 6 years . This has to be added to the delta V required to maintain inclination and to correct launcher injection errors (estimated between 10 m/s and 20 m/s depending on the launcher). A total of 40 m/s is assumed.

Even for maximum along-track drift the angular depointing of MASTER with respect to the METOP velocity will be 1 deg, well within the swath of the METOP instruments. OMI/GOME, IASI and AVHRR will also overlap sufficiently with MASTER at the poles when the MASTER line-of-sight is intentionally depointed by 10 deg.

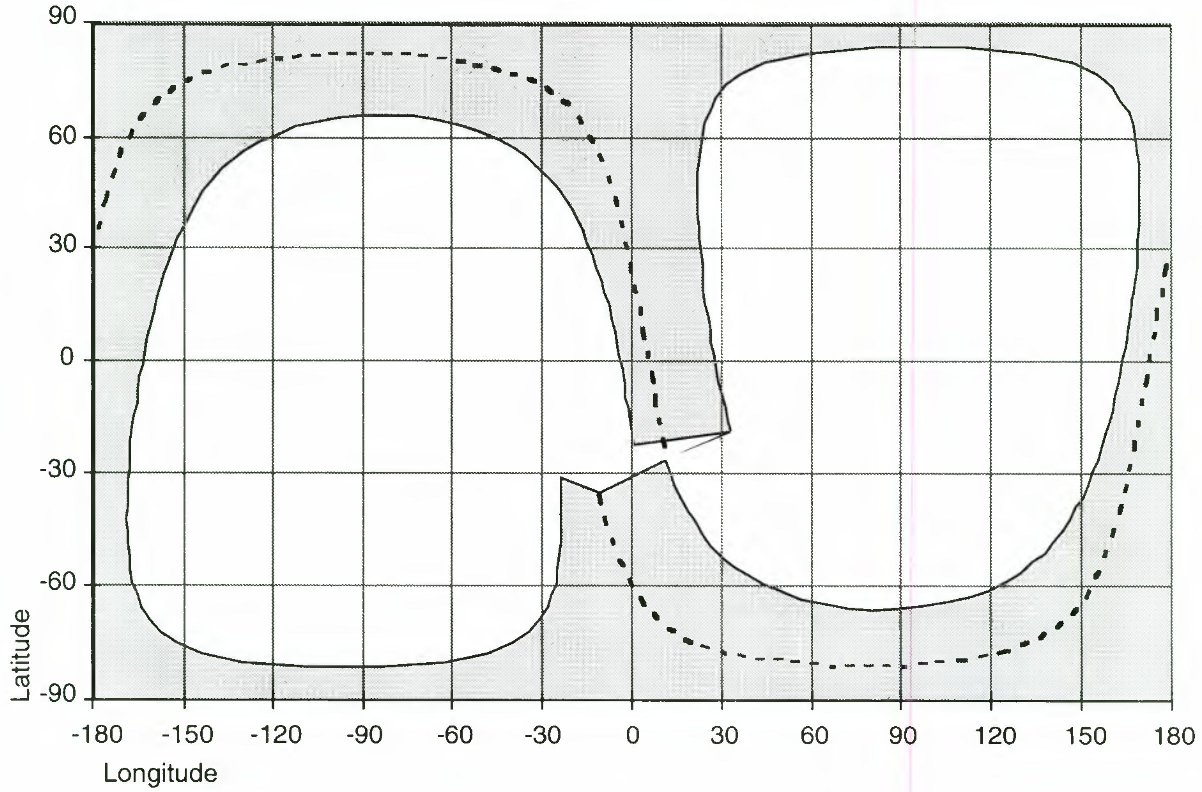


Figure 6.8. *Coordination with ENVISAT: The greyed area shows the accessible range of the MIPAS instrument on ENVISAT during one (arbitrary) orbit. The dotted line shows the observations of the MASTER instrument on ACE, which lies clearly inside the range of the MIPAS instrument and therefore represents one orbit of possible common observations of the same target. 12 consecutive orbits (not represented here) cover almost the entire earth.*

Simultaneous observations with MIPAS are also possible if ACE is coincident with the second half of ENVISAT's operational life. MIPAS operations on ENVISAT could be planned to have the MIPAS line-of-sight targeting the atmosphere volume observed by MASTER. If only MIPAS observations, performed within 6 minutes before or after MASTER observations, are considered, there would be 4 sets of 12 orbits (i.e. 48 in all) within every ENVISAT 3 day cycle, (i.e. 48 orbits of concurrent MASTER – MIPAS measurements). The principle is illustrated in figure 6.8 which shows that the MASTER track would lie within reach of the MIPAS pointing capabilities.

The operational concept is simple as only one repeated operational sequence is foreseen. At a certain latitude in each hemisphere, the instrument itself or the platform would be pointed in azimuth 10 deg to the right or the left to observe the adjacent pole. The operation is automatically commanded on-board based on the navigation information provided by GRAS. This azimuth scanning can be inhibited from ground.

The satellite is earth pointed. No attitude manoeuvres are required, except for orbit corrections which, as shown above, should be very infrequent. Slew manoeuvres could be also considered for the 10 deg depointing to observe the poles.

The contact times in minutes with some European ground stations, representative of different latitudes, are summarised below.

	per day	per orbit average	minimum per orbit	maximum per orbit	% visible orbits
Svalbard	149	10.4	5.5	12.5	100
Kiruna	110	10	2.25	12.5	74
Fucino	49	3.44	2	12.25	35

The tandem operation with METOP is possible without additional workload on satellite control as METOP and ACE would be controlled by different organisations from different centres and ground stations. Coordination would certainly be required. The coordination of observations with MIPAS should not affect the ACE.

6.4. Spacecraft

6.4.1. Configuration

The successful platforms of the Mark series used for ERS, SPOT, METOP, Helios would be oversized for ACE. A smaller satellite would suffice. Its conceptual configuration is driven by the accommodation of the 2 m antenna of MASTER and by launcher constraints. Candidate configurations are shown in figures 6.9 and 6.10. Configuration A (figure 6.9) would require a thermal shield to shadow the MASTER antenna. This shield could be conveniently used to install some of the MASTER units. Configuration B (figure 6.10) installs the instrument on the antisun side. Concept studies on the candidate Earth Explorers show the possibility of using the same type of platform for both ACE and for the Earth Explorer Surface Processes and Interactions Mission.

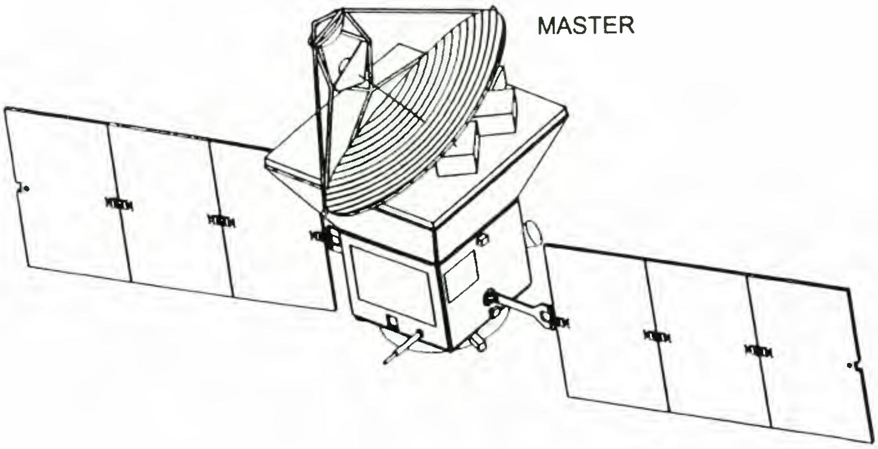


***Figure 6.9**. ACE configuration concept A*

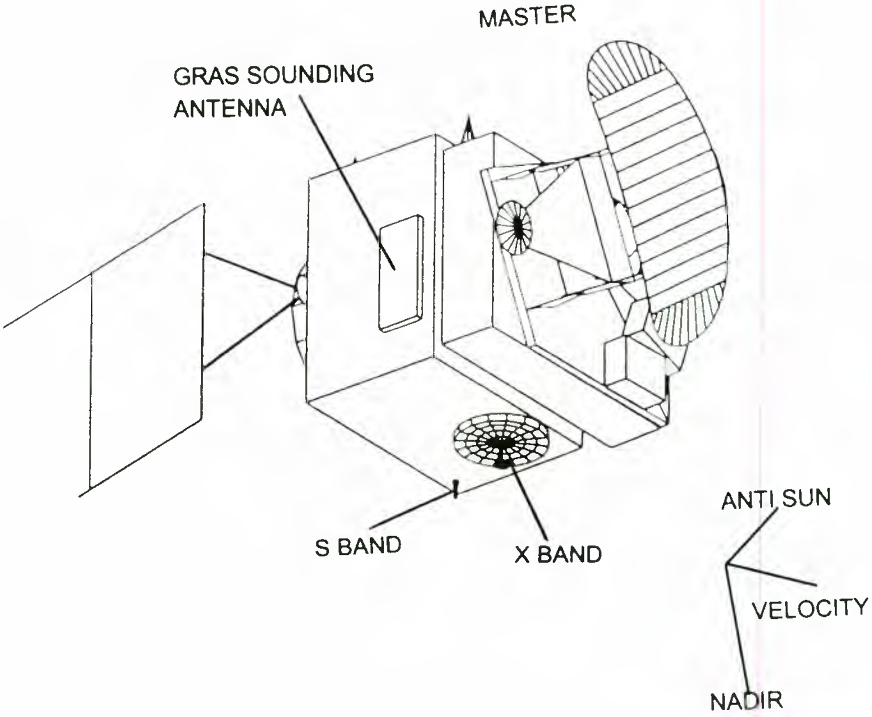


***Figure 6.10**. ACE configuration concept B*

6.4.2. Mechanical and Propulsion Systems

The proposed structural concept is classical. First analyses indicate its suitability for the environment of Ariane 5 or small launchers.

The mechanisms foreseen include on payload side, the scanning of MASTER in elevation and possibly also for its orientation in azimuth (if not provided by the platform). The disturbances introduced will be compensated at instrument or platform level. At platform side only the deployment and orientation of the solar array require mechanisms.

The thermal control concept is passive. The platform proper consumes less than 200 W of power which must be compared with the 600 W that can be dissipated at the proposed orbit with the available radiating area. MASTER is autonomous from the thermal control point of view. The dissipation of payload data management and communications equipment are estimated to be around 50 W including margin. This is well below the radiating capabilities offered by the satellite and allows the MASTER electronics (less than 200 W) to be accommodated inside the platform.

The proposed propulsion concept is based on standard components and uses hydrazine with 16 kg are necessary to provide the 40 m/s of required delta V for the reference satellite mass. 20 kg are loaded on-board to provide margin.

6.4.3. Electric Power

The electric power system in the configuration shown in figure 6.9 has a solar array composed of two wings of 4 m^2 each of GaAs solar cells with efficiency better than 150 W/m^2. The 1200 W generated are enough to supply the satellite and charge the 40 Ah battery which in turn provides electric power during the eclipse. The concept of figure 6.10 includes a single solar wing of the same total capability.

6.4.4. Attitude and Orbit Control

The Attitude and Orbit Control System (AOCS) concept estimates and controls the satellite orbit and attitude.

Orbit control would depend on the maintenance of the tandem with METOP but will be infrequent (see earlier). Orbit and attitude estimation are driven by observation geolocalisation requirements. The most demanding requirement is the vertical localisation of MASTER observations. However, as MASTER includes its own star sensor, the task of the platform is reduced.

Concerning attitude control a 0.6 mrad accuracy, equivalent to 2 km at the limb, is considered sufficient to allow MASTER's scanning mechanism to cover the area of interest in elevation. Better pointing accuracy would allow the more efficient use of the scanning range of MASTER.

Attitude rate stability is driven by the requirement to preserve MASTER observation quality. A requirement of 200 microrads/s below 1 Hz has been imposed. This corresponds to 10% of the elevation scanning velocity. Stability along the complete elevation scan would mean a more demanding requirement but would result in even better observation quality.

Orbit determination is based on GRAS (ESA,1996b), which provides in real-time an accuracy of 50m enabling autonomous azimuth manoeuvres. This accuracy is also enough for the geolocalisation of the observations but can be improved after processing so that nearly the complete geolocalisation error allowance could be allocated to attitude restitution.

For attitude estimation the proposed implementation includes gyros and star sensors. For acquisition and safe mode sun sensors and a magnetometer are proposed.

Reaction wheels and magneto-torquers are used for attitude control. A possible implementation could include reaction wheels of 25 Nms and magneto-torquers of 140 Am^2.

6.4.5. Command and Data Handling

The Command and Data Handling System concept performs the platform command and data handling and the payload data handling functions. The proposed platform data handling is conventional and structured around a serial bus like ESA OBDH bus. A single on-board computer is capable of handling all satellite tasks including AOCS and payload interface tasks. Time reference is provided by GRAS ensuring a datation to UTC better than fractions of ms. As METOP is also expected to carry GRAS, so the synchronisation of ACE and METOP observations to UTC could be automatically achieved to the order of the millisecond.

MASTER is connected to the serial bus for command and control with the science data being supplied in the form of source packets to a solid state memory recorder via a dedicated link.

The data generation is less than 500 kbps assuming overheads and R-S coding, i.e. 3 Gb per orbit. A 15 Gb solid state memory recorder is foreseen to store all data generated on-board between contacts with the ground station, including blind orbits. A downlink data rate of at least 10 Mbps would allow the dumping of the stored data to a station like Kiruna.

Figure 6.11 shows the functional architecture of the ACE avionics concept. The connections do not represent actual hardware connections.

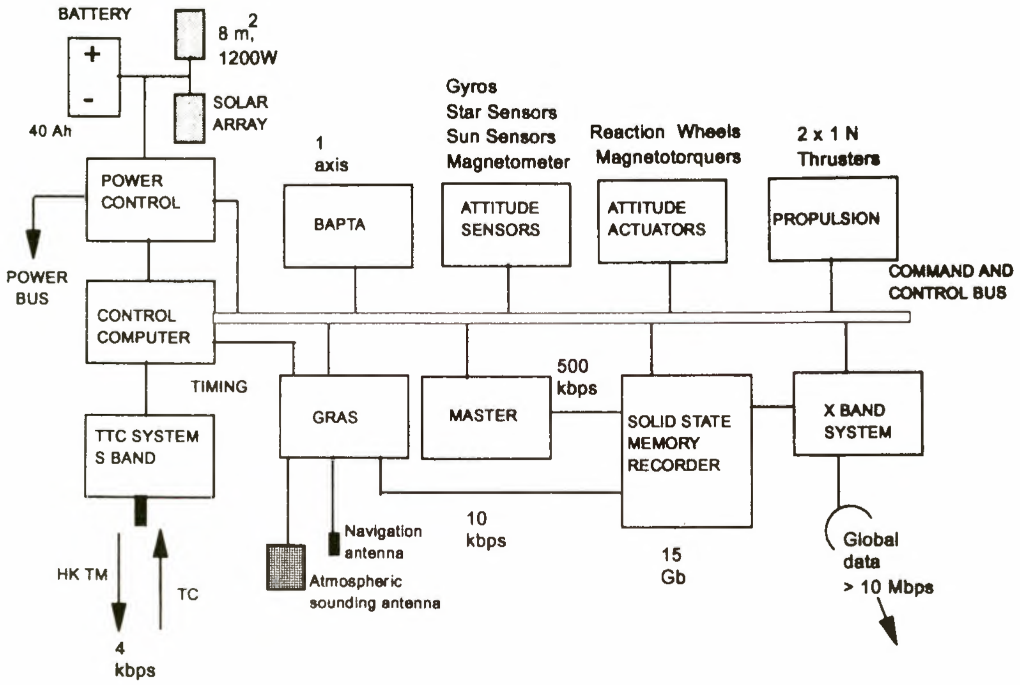


Figure 6.11. Functional architecture of ACE avionics

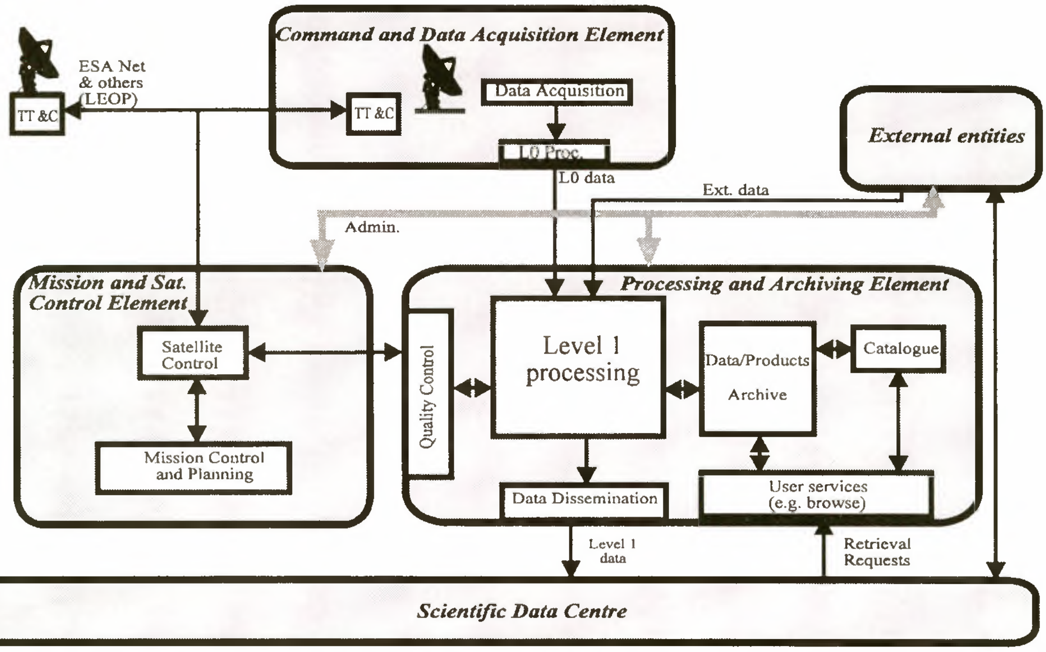


Figure 6.12. Ground segment architecture

6.4.6. Communications

The communications system concept includes both the S band and the X band assemblies. The S band is used for telecommand and housekeeping telemetry. The telecommand link is at 2.07 GHz at a rate of 4 kbps. The telemetry link at 2.24 GHz handles also 4 kbps.

The X band system (8.4 GHz) is used for delivery of the global data stream: science and satellite data. It performs the formatting and modulation and the actual transmission to ground. The downlink data rate must be at least 10 Mbps.

6.4.7. Satellite Budgets

The satellite budgets for the Atmospheric Chemistry Explorer concept for the various systems have been indicated above. The overall (i.e. ACE) satellite mass and power budgets are estimated to be:

Mass (kg)		*Power (W)*	
Payload	350	Payload	400
Payload Module	80	Payload Module	50
Platform	280	Platform Service	140
Dry Mass	710	Subtotal Satellite	590
With 10% Margin	780	With 10% Margin	650
Propellant	20	Losses	50
Total	*800*	*Total*	*700*

6.5. Ground Segment and Data Processing

6.5.1. Overview

Figure 6.12 shows an overview of the ground segment. It includes 3 main elements, the Command and Data Acquisition Station, the Mission and Satellite Control Element, the Processing and Archiving Element and the Science Data Centre that are summarily described below. The expected available infrastructure around the year 2003, with appropriate adaptation, should be enough to support this mission and ENVISAT simultaneously. METOP will be controlled by Eumetsat with a separate ground segment. No problems are anticipated to handle the proposed mission baseline including ACE and the synergy with METOP and ENVISAT.

The following processing levels are identified:

- Level 0, raw data, time ordered and without overlaps;
- Level 1a, data 'depacketised', calibration and geometric corrections computed and appended but not applied;
- Level 1b, data with calibration and geometric corrections applied and geolocalised;
- Level 2, geophysical variables.

6.5.2. Command and Data Acquisition Station

A single European ground station (e.g. Kiruna) would be sufficient as Command and Data Acquisition Element. The station would perform data acquisition and satellite command. The 10 Mbps data downlink could be easily handled. At the date of the mission the ERS reception system could be used. The station would also provide processing to level 0 and short term data buffering for typically one week.

6.5.3. Mission Operations and Satellite Control Element

This element will perform the monitoring and control of the mission operations and of the satellite including payload and will monitor the operation of the ground segment itself. This element would be also in charge of coordination with the METOP ground segment and would ensure the coordination with ENVISAT for the planning of MIPAS observations. No really demanding requirements have been identified for the communication between the various elements of the ground segment.The simplicity of the operations and the classical autonomy of the satellites are such that very little interaction between ground control and the satellite is expected. Command sessions could be planned every week. Telemetry will be automatically analysed after receipt and alarms would be automatically triggered after analysis.

6.5.4. Processing and Archiving Element

The data would be processed to Level 1a/1b by the Processing and Archiving Element and would then be sent to the Science Data Centre.

Data would be archived at Level 1a for a period extending until 10 years after the mission. Archived data should be catalogued and a browsing facility could also be envisaged to support user access to the archive.

6.5.5. Data Processing

The MASTER Level 1b processing would consist basically of radiometrically calibrated spectra. Only instrument related data would be required. Absolute and relative position and pointing information would be extracted from the platform AOCS (including GRAS) and from MASTER spectra. Level 2 processing would be based on a non-linear least square fit of MASTER spectra to a radiative transfer model. Large experience exists from previous limb sounder missions and additional work is currently ongoing in scientific institutes to ensure the retrieval of data even in presence of cirrus clouds.

There is a great potential to increase accuracy, altitude range and validity of the geophysical data by merging data from the involved instruments onboard ACE and METOP. A full exploitation of these data would require a data assimilation system.

6.6. Launcher Considerations

Ariane 5 is indeed capable of launching ACE in dual launch configuration if suitable partners are found. If dedicated launchers are considered, the most attractive (from the cost point of view) is Eurockot. It is however marginal in terms of volume under fairing and some tens of kg short in performance with the current ACE mass estimates if launch from Plesetsk is assumed and safety constraints are not waived. As alternative the American LLV2 has been considered.

6.7. Implementation Options

One option considered includes MIPAS with MASTER on the same platform. The mission profile is the same as for the baseline with MASTER alone. MASTER would be unchanged in the essentials but the configuration may have to be adapted as present concepts were designed for accommodation on the anti-sun side of the platform which also be required by MIPAS. The description of this option is therefore limited to considerations on the main characteristics of MIPAS and the introduction of the spacecraft concepts. A second option consists of implementing an additional receiver in MASTER to detect HCl.

6.7.1. MASTER – MIPAS

MIPAS

MIPAS is a Fourier transform spectrometer used as a passive radiometer in the mid-infrared range. It covers the region between 685 and 2410 wavenumbers (4.15 to 14.6 μm) with 2 groups of 4 detectors (one photoconductive and two photovoltaic HgCdTe, and one photovoltaic InSb), with a spectral resolution of 0.05 wavenumber. Some redundancy in the detecting scheme, as well as optimisation of the sensitivity, are achieved by using the two output ports of the interferometer. The detectors are actively cooled to 70 K. The instrument itself is kept at about 210 K. Similar to MASTER, MIPAS has an internal hot load and uses cold space for calibration. MIPAS makes a limb measurement in about 4 s.

Its field-of-view is 3 km vertically and 30 km horizontally. A complete elevation scan lasts about 1 minute. MIPAS has the capability to look in two azimuth ranges: antiflight and across track. This capability would be used to coordinate its observations with those of MASTER.

Spacecraft

The satellite could use a platform of the Mark series used by SPOT, ERS and METOP. A possible configuration is shown in figure 6.13.

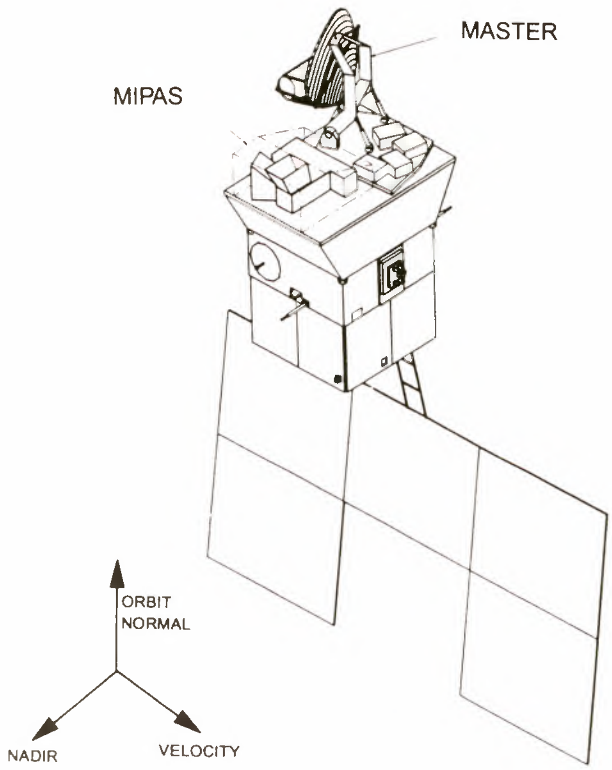


Figure 6.13. *MASTER- MIPAS option, configuration based on ERS/SPOT type platform*

Alternatively dedicated optimised concepts can be envisaged. A potential implementation is shown in figure 6.14. This configuration takes advantage of the fact that both instruments are limb sounders so the nadir face could be small and a larger anti-sun side can be provided. This would result in a more compact and lighter satellite, around 10% mass savings, compared with the Mark based option. The MIPAS – MASTER option is described below in comparative terms with respect to the baseline:

The payload mass would go from 350 kg to 630 kg, the power requirements from 400 to 570 W, and the data rate from 500 kbps to 1200 kbps. In addition, the required accommodation foot print and volume would increase. Space and ground segment would be proportionally more complex.

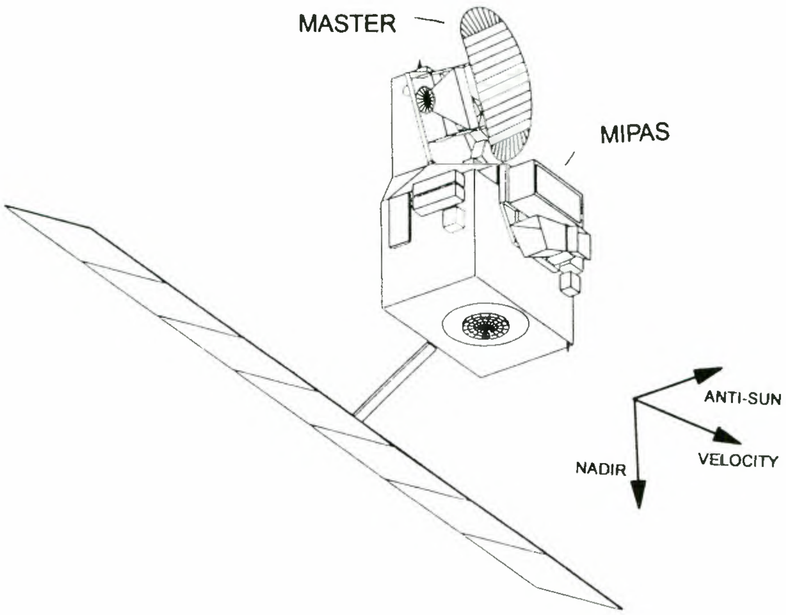


Figure 6.14. *MASTER - MIPAS option on dedicated platform*

The AOCS requirements would be unchanged as MASTER is more demanding than MIPAS in terms of attitude control, stability and estimation requirements. The disturbances would be larger and the actuators would have to provide higher torque and momentum storage capability. However, the standard ERS equipments could be used. The propulsion system could also use the standard ERS, SPOT units. A two tank configuration would have to be utilised.

The overall mass and power budgets are:

Mass (kg)		*Power (W)*	
Payload	630	Payload	570
Payload Module	110	Payload Module	70
Platform	850	Platform Service	320
Dry Mass	1590	Subtotal Satellite	960
With 10% Margin	1750	With 10% Margin	1060
Propellant	150	Losses	90
Total (Approx.)	*1900*	*Total*	*1150*

The launcher could be for example Delta or LLV3. Shared launch with Ariane 5 has also been considered.

6.7.2. Additional HCl Channel

An additional channel can be implemented on MASTER to allow detection of HCl. The most important impacts on the instrument design are estimated to be a 15% increase in mass, power consumption and data rate and a higher complexity of the quasi-optics. Because of the high frequency (625 GHz) of this channel, the development risks and costs of certain assemblies would increase: i.e. antenna (reflector surface accuracy and subsystem verification), mixers and local oscillators. The higher mass, power and data rate of the instrument will have associated effects on the satellite and the ground segment.

7. Programmatics

7.1. General

The Earth Explorer Atmospheric Chemistry Mission would be implemented in the frame of the ESA Earth Explorer Programme of research missions if selected after phase A studies carried out within the frame of the Agency's Earth Observation Preparatory Programme.

7.2. Critical Areas and Open Issues

The Earth Explorer Atmospheric Chemistry mission has been defined based on the in orbit presence of METOP carrying OMI/GOME and IASI and certain assumptions have been made on their performances. Changes in METOP could affect the definition of the Earth Explorer Atmospheric Chemistry Mission.

The definition of the core Atmospheric Chemistry Mission has been based on the availability of a significant increase in knowledge of NO_x chemistry (due to ENVISAT) or on the simultaneity of the Explorer and ENVISAT. Changes in these assumptions would affect the definition of the Explorer. The various options have therefore been studied in some detail as described in chapter 6.

From the technical point of view MASTER is a challenging instrument but suitable concepts have been developed in pre-phase A activities so the risk is small.

A robust technology effort has already been in progress for several years including developments in the areas of antennas (and their verification techniques), receivers, spectrometers, and mechanisms. Though difficult, the criticalities have been identified and do not appear to be insurmountable.

The core mission could be implemented on a small platform which could benefit from the large heritage with Earth Observation platforms and from the several initiatives currently under way in Europe. No problems are expected.

The ground segment should not present any critical area and the infrastructures set up for ERS and ENVISAT should suffice technically.

7.3. Related Missions and Timeliness

The Earth Explorer Atmospheric Chemistry Mission is intimately related to METOP, not only for the 'objective analysis' of the conventional meteorological data, but also for the use of the observations of OMI/GOME and IASI and the identification of cloud coverage with AVHRR. The Earth Explorer Atmospheric Chemistry Mission would utilise METOP chemistry observations and at the same time multiply the scientific return of these observations.

The Earth Explorer Atmospheric Chemistry Mission also relates to ENVISAT whose value would be enhanced by complementing the measurements made by MIPAS and SCIAMACHY. MIPAS would provide information on the NO_x terms in the ozone budget equation.

The above considerations affect the timeliness of the mission which should be in orbit around the year 2003 to be coincident with METOP and still overlap the second half of the ENVISAT mission while at the same time benefiting from the exploitation of GOME on ERS-2, and of the initial years of OMI/GOME, IASI and MIPAS.

The Earth Explorer Atmospheric Chemistry Mission fits in the international scenario formed by the Japanese ADEOS (ADEOS III in 2002) and the American EOS-CHEM missions and would build on the heritage of European missions such as ODIN and the AMAS flight on Meteor. The Earth Explorer Atmospheric Chemistry Mission will be a bridge to the Japanese ATMOS- C1 (2006) with its suite of related instruments such as MILES, ILAS III, etc.

7.4. International Cooperation

European cooperation is intrinsic to the definition of the mission which uses the observations of METOP. The potential flight of AMAS on Meteor could be a precursor and in fact there is potential for the harmonisation of the AMAS and MASTER developments.

The synergies between the Earth Explorer Atmospheric Chemistry Mission and the EOS CHEM mission of NASA could lead to cooperation with coordination on platforms and instruments.

The similarities and complementarities with the Japanese ATMOS-C1 mission also offer good possibilities for international cooperation.

7.5. Enhancement of European Capabilities and Applications Potential

The Earth Explorer Atmospheric Chemistry Mission would endow Europe with new and complementary observation capabilities for chemistry and climatology built on MASTER, OMI/GOME and IASI, SCIAMACHY and MIPAS.

The potential cooperation established within Europe and with NASA and NASDA could contribute to future collaborative ventures.

The development of MASTER would consolidate Europe's position in the area of the mm and sub-mm technologies.

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Acronyms

ACE	Atmospheric Chemistry Explorer
ADEOS	Advanced Earth Observing System
AOCS	Attitude and Orbit Control System
AVHRR	Advanced Very High Resolution Radiometer
CFCs	Chlorofluorocarbons
ENVISAT	ENVIronmental SATellite
ERS	European Remote Sensing satellite
EUMETSAT	EUropean METeorological SATellite agency
GNSS	Global Navigation Satellite System
GOME	Global Ozone Monitoring Experiment
GOMOS	Global Ozone Monitoring by Occultation of Stars
GPS	Global Positioning System
GRAS	GPS/GNSS Receiver for Active Stratospheric Sounding
HEMT	High Electron Mobility Transistor
IASI	Infrared Atmospheric Sounding Interferometer
IF	Intermediate Frequency
ILAS	Improved Limb Atmospheric Spectrometer
IMG	Interferometric Monitor for Green house Gases
IPCC	International Panel on Climate Change
KNMI	Koninklijk Nederlands Meteorologisch Instituut
LS	Lower stratosphere
MASTER	Mm-wave Acquisitions for Stratospheric/Tropospheric Exchange Research
METOP	METeorological OPerational satellite
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
MOPITT	Measurements of Pollution in the Troposphere
OBDH	On-Board Data Handling
ODIN	The name of a Norwegian Space Mission
OMI	Ozone Monitoring Instrument

PAN	Peroxyl Acetyl Nitrate
PSC	Polar stratospheric cloud
SAGE	Stratospheric Aerosol and Gas Experiment
SBUV	Solar backscatter ultraviolet instrument
SCIAMACHY	SCanning Imaging Absorption Spectrometer for Atmospheric CartograpHY
SPOT	Satellite Pour l'Observation de la Terre
STE	Stratospheric/Tropospheric Exchange
TOMS	Total Ozone Mapping Spectrometer
UARS	Upper Atmosphere Research Satellite
UT	Upper Troposphere
UTC	Universal Time Coordinated
UV	UltraViolet radiation
WMO	World Meteorological Organisation

European Space Agency
Agence spatiale européenne

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