

**Chapter 1:**  
**General Introduction**

# Chapter One

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### 1.1 Overview

The exchanges of momentum, heat, water vapour and carbon dioxide between the atmosphere and the surface of the Earth are the primary mechanisms by which the surface responds to and modifies the climate of the Earth. These exchanges occur over a wide range of space and time scales, from molecular to global and from milliseconds to decades and they are quantified by flux densities, the amount of momentum, energy or mass moved across a unit area per unit time. The term "flux densities" is often shortened to simply "fluxes" and this convention is followed here.

The fluxes of energy and mass are vectors with three components while that of momentum is a second order tensor with nine components. Further, it is often useful to consider all components of the fluxes as consisting of mean and fluctuating parts, corresponding to advection and turbulent transport respectively. This brings the number of terms needed to fully describe the fluxes of momentum, heat, water vapour and carbon dioxide to 36, which suggests that some simplification will be required before progress can be made toward understanding the important processes. The simplification adopted here is twofold. Firstly, only the vertical component of the fluxes will be considered and secondly, only the turbulent transport will be examined. The number of terms in the total fluxes is then reduced from 36 to four.

The above simplifications are justified on the basis of two assumptions. Firstly, that the flow field, and hence the underlying surface, is horizontally homogeneous and secondly, that the mean vertical velocity near the ground is zero (Finnigan et al., 2003; Stull, 1988). The first assumption conveniently removes the possibility of horizontal gradients in the means, variances and covariances thereby ensuring the horizontal advective and turbulent fluxes are zero. The second assumption removes the vertical advective flux components. The validity and consequences of these assumptions has been the subject of some discussion in the recent literature (Sakai et al., 2001; Massman and Lee, 2002; Finnigan et al., 2003) and is not pursued here. Rather, the simplifications are made in order to progress and then form the background against which the results of the current work are interpreted. Within this

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context, the term "fluxes" is used here to mean the vertical component of the turbulent fluxes at the surface.

Knowledge of the fluxes is important for many reasons. The flux of sensible heat determines the stability and growth of the atmospheric boundary layer and this is used, for example, to predict levels of air pollution. The flux of water vapour can be directly used by agronomists to assess the water loss by crops and hence their irrigation needs. The ratio of carbon dioxide uptake to water vapour loss can be used as a basis for selecting cultivars in breeding programmes in order to improve crop yield or reduce water use. The flux of carbon dioxide (CO<sub>2</sub>) is a direct measure of net ecosystem exchange and quantifies the transfer of carbon between atmospheric, terrestrial and oceanic stores. This is of particular interest given the current concern about rising CO<sub>2</sub> concentration in the atmosphere and the uncertainties in the sequestration of carbon in the terrestrial biosphere (Houghton, 2003).

Energy and mass fluxes also influence the weather and climate directly, through the transfer of heat and water vapour into and out of the atmosphere, and this involves an important feedback. The local climate is heavily influenced by the partitioning of energy at the surface into the fluxes of heat and water vapour. This is largely controlled by the nature of the surface vegetation which itself responds to the local climate either by modifying its own behaviour or, at long time scales, by migration. Through this direct influence on the weather and climate, the fluxes form the lower boundary conditions for general circulation models (GCM) and the processes controlling these fluxes need to be understood in order to predict their magnitude and improve the accuracy of climate forecasts. Understanding of these processes is also required in order to predict how they will change in response to a changing climate.

The fluxes of energy, mass and momentum occur across a range of length and time scales. Those interactions occurring at the regional scale, of order 100 km, are of particular interest. This scale falls between the patch scale, of order 100 m, which is accessible by traditional micrometeorological techniques, and the continental scale, of order 1000 km, which is accessible by inversion techniques (Gurney et al., 2003; Wang and McGregor, 2003). Several important processes occur at the regional scale and their investigation is hampered by the lack of suitable experimental techniques.

Examples of these processes are evaporation from whole catchment areas (Cleugh, 1991; Chehbouni et al., 2000) and carbon uptake by whole ecosystems (Schimel et al., 2001). The horizontal resolution of current GCMs also falls into the regional scale, information is required at this scale for input and for validation (Sellers et al., 1996a; Garratt et al., 2002). Information on trace gas exchange at the scale of whole ecosystems also makes a convenient building block from which to assemble continental scale emission inventories (Galbally et al., 1992).

This thesis considers the estimation of regional scale fluxes of heat, water vapour and CO<sub>2</sub> by combining meteorology observed at a centrally located point with spatially resolved surface properties. The meteorological variables provide the temporal forcing for the fluxes while the spatially resolved surface properties describe the spatial forcing of the fluxes by the surface heterogeneity. The literature abounds with schemes for aggregating leaf scale observations to whole canopies (Jarvis and McNaughton, 1986; Kim and Verma, 1991; McNaughton and Jarvis, 1991; Lhomme, 1992; McNaughton, 1994; Raupach, 1995). The canopy to region transition has also received considerable attention (Braden, 1995; Michaud and Shuttleworth, 1997; Hasager and Jensen, 1999; Hu et al., 1999; Anderson et al., 2003). However, much of the reported work is concerned with modelling and less is directed towards observational, or even integrated modelling and observational approaches. Regional scale observations of the fluxes are usually available only during special observing periods from networks of instrumented towers (Smith et al., 1992; Soegaard, 1999; Baldocchi et al., 2001a; Mahrt et al., 2001) or the flights of research aircraft (Desjardins et al., 1992a; Ogunjemiyo et al., 1997; Gottschalk et al., 1999; Bange et al., 2002). The work described here is a contribution toward current efforts at filling this gap in observations of surface-atmosphere interaction at regional scales.

The data used in this thesis come from the Observations At Several Interacting Scales (OASIS) experiment, a multi-disciplinary land-atmosphere interaction study conducted in southern New South Wales, Australia, in the austral springs of 1994 and 1995 (Leuning et al., 2004). In both years, observations were made over a three-week period at six (1994) or eight (1995) ground-based sites, from research aircraft, from free-flying and tethered balloon systems and from satellites. The OASIS experiment is described fully in Chapter Two.

## 1.2 General Concepts and Topics

### 1.2.1 Atmospheric Boundary-layer

The topics covered in this thesis are confined to the atmospheric boundary layer (ABL). The ABL is defined as "that part of the troposphere that is directly influenced by the presence of the earth's surface, and responds to surface forcing with a time scale of about an hour or less" (Stull, 1988). The depth of this layer is typically 1-2 km during the day and up to a few hundred metres during the night. The contact with the surface and the diurnal cycle in surface heating driven by the Sun's passage across the sky are fundamental determinants of the state of the ABL. But underlying these states is the generation of turbulence as shear forces overcome viscosity when air passes over a rough surface. Since the air is never completely at rest, the ABL is characterised by turbulence and the state of the ABL can be described by the extent to which the generation of turbulence by shear is enhanced or suppressed.

During the day, energy from the Sun warms the surface and, by conduction, the air in contact with the surface is warmed. At some point, this air, less dense than the air above it, separates from the surface, convection takes over and the parcel of air rises until the buoyancy forces again balance. The importance of convection in the daytime ABL is indicated by the name adopted for this state of the ABL, the convective boundary layer (CBL). In the CBL, shear generation of turbulence is enhanced, complemented, and at times dominated by the production of turbulence by buoyancy forces. During the night, longwave radiation cools the Earth's surface and the air in contact with it, establishing a stable density gradient in the lowest layers of the ABL. In this state, buoyancy forces suppress the production of turbulence by wind shear and, at the extreme, turbulence can become intermittent. This state is variously called the stable boundary layer (SBL) or the nocturnal boundary layer (NBL), the latter reflecting the fact that stable conditions occur most frequently at night.

The work described in this thesis focuses on processes occurring in the CBL and, in particular, on the period from two hours after sunrise to two hours before sunset

when the CBL depth is increasing or steady. This is also the period when the time scale of surface exchange processes is significantly less than the time scale of the CBL and for the purposes of studying these exchanges, the CBL can be considered quasi-stationary. This concentration on the CBL does not imply that processes occurring in the SBL are of lesser importance, only that they lie outside the scope of the current work.

The basic structure of the CBL can be described by reference to several sub-layers. Closest to the surface and extending up to three times the vegetation canopy height is the roughness sub-layer where the flow is still influenced by individual roughness elements (Kaimal and Finnigan, 1994).

Above the roughness sub-layer is the surface layer. The vertical extent of the surface layer has been variously defined as one tenth of the ABL depth, the depth of the "constant flux" layer (more rigorously, the height at which the fluxes have decreased by 10% from their surface values) or some multiple of the Monin-Obukhov length,  $L$ , defined as:

$$L = -\frac{\rho c_p \theta u_*^3}{kgF_H} \quad 1.1$$

Here  $\rho$  is the air density,  $c_p$  is the specific heat at constant pressure,  $\theta$  is the potential temperature,  $u_*$  is the friction velocity,  $k = 0.4$  is von Karman's constant,  $g$  is the acceleration due to gravity and  $F_H$  is the sensible heat flux. The definition for the depth of the surface layer adopted here is  $z \leq |L|$  based on the observation that shear production of turbulence is dominant for heights up to  $|z/L| \approx 1$  (Kaimal and Finnigan, 1994).  $z$  is the height above the surface.

Above the surface layer, at heights between  $|L|$  and one tenth of the ABL height, is the convective matching layer where the profiles of wind and scalars are in transition between their forms in the surface layer and those in the mixed layer. Within the mixed layer,  $0.1z_i$  to  $z_i$ , where  $z_i$  is the depth of the ABL, buoyancy forces are dominant over shear forces and the profiles of wind and scalars become constant with height due to vigorous vertical mixing. The entrainment zone is often

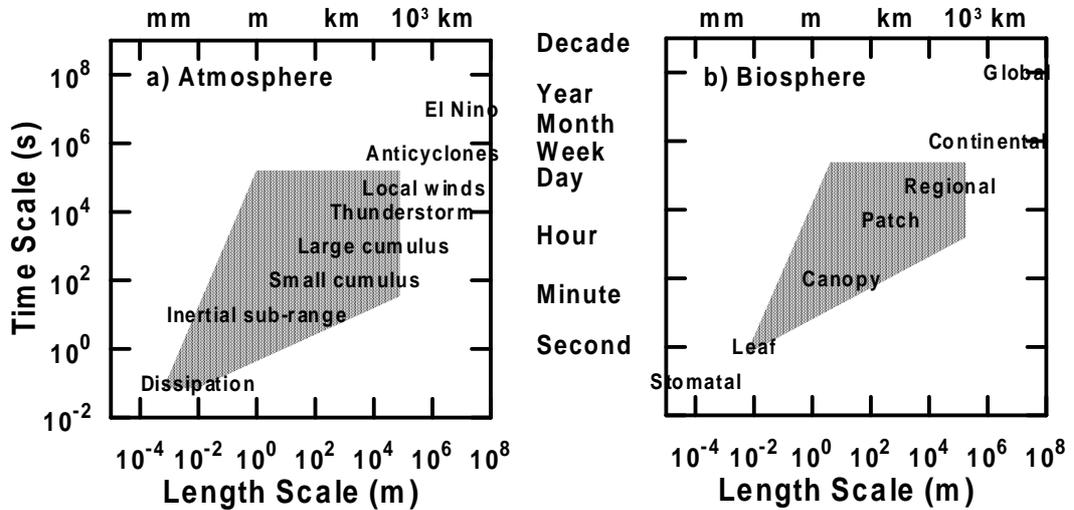
characterised by sharp transitions in the wind and scalar values and separates the mixed layer from the free troposphere above it. This zone and the associated temperature inversion at  $z_i$  form the upper limit of the boundary layer. Kaimal and Finnigan (1994) provide a good description of the sub-layers comprising the ABL, the scaling parameters and the relative behaviour in each of mean values and turbulent fluxes with height.

### 1.2.2 Length and Time Scales

The processes responsible for the surface-atmosphere exchange of heat, moisture and CO<sub>2</sub> in the ABL occur over a wide range of space and time scales. These are summarised in Figure 1.1.

The depiction of scales in the atmosphere (Figure 1.1a) has been truncated for ease of display. In reality, the upper limit on the spatial scale is of the order of the diameter of the Earth and the upper limit on the temporal scale is millennia due to the variability of the Earth' s climate. The discussion here starts at the top right hand corner with quasi-annual climatic features such as El Nino, which have spatial scales of the order of  $10^4$  km and time scales of about one year. The next major grouping, not shown in Figure 1.1a to avoid clutter, are the four seasons that result from the Earth' s orbit around the Sun and the inclination of the Earth' s axis of rotation with respect to the orbital plane. Below this, with time scales of a week and spatial scales of  $10^3$  km, come the synoptic weather patterns associated with cyclones and anticyclones. Next in this cascade of scales are local winds (eg sea breezes, land breezes, katabatic winds etc), often referred to as mesoscale flows, with spatial scales of a few hundred kilometres and time scales of a day or so. These phenomena form the upper limits of those processes directly represented in the structure of the ABL but it is important to recognise that all ABL processes occur against the backdrop of, and are influenced by, synoptic, seasonal and climatic variability. Within the scales commonly observed in the ABL come cumulus clouds and the production of turbulence by shear and buoyancy forces. Most significant for the ABL is the cascade of turbulent energy from production at scales of a few hundred metres to dissipation by viscous forces at scales of millimetres. It is the turbulent motions

within this cascade that provide the mechanism for surface-atmosphere exchange of heat, moisture and trace gases.



**Figure 1.1** Schematic diagrams of length and time scales in a) the atmosphere and b) the biosphere. Figure 1.1a has been re-drawn from Oke (1987) and the shaded area indicates the range of space and time scales encountered in the ABL. The shaded area in Figure 1.1b indicates the approximate range of space and time scales covered by the OASIS experiments.

A similar diagram can be drawn for the biosphere and this is shown in Figure 1.1b. The shaded region in Figure 1.1b indicates the length and time scales sampled during the OASIS experiments. The scales investigated during OASIS ranged from individual leaves ("leaf") to individual plants ("canopy") to homogeneous crop or pasture fields ("patch") and up to a region of 130 by 50 km ("regional").

Measurements of leaf gas exchange are made on individual leaves at length scales of 1 to 10 cm and time scales of seconds to minutes. These data provide information on the stomatal resistance to gaseous diffusion between the leaf interior and the air in contact with the leaf surface. The canopy resistance can then be obtained by integration of the stomatal resistance over the leaf area of the canopy; this is the classic method of upscaling results from leaf to canopy scales. Leaf gas exchange observations can also provide data on net photosynthesis, the amount of CO<sub>2</sub> fixed by gross photosynthesis minus the CO<sub>2</sub> lost by respiration (Oke, 1987).

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The canopy has length scales of the order of metres and time scales of the order of minutes. Measurements of gas exchange between the soil and the boundary-layer due to heterotrophic and root respiration can be made by individual chambers. Stacked chambers, enclosing a whole plant, can be used to measure both autotrophic and heterotrophic respiration (Meyer et al., 2001). Patch scale measurements are provided by standard micrometeorological techniques (Kaimal and Finnigan, 1994). The source area at the surface determines the length scales of these observations with typical values of a few hundred metres for short towers in unstable conditions (Horst and Weil, 1992). The time scale is the averaging period for the observations, usually between 15 minutes and 1 hour.

Regional processes are characterised by length scales of hundreds of kilometres and time scales of hours and several measurement techniques provide data at these scales. Networks of ground-based sites can provide information on the regional scale variability in the fluxes of heat, moisture and CO<sub>2</sub> but each site is representative of a limited area. Instrumented aircraft flying at low altitudes provide observations of the fluxes and mean meteorological quantities over distances of 100 km in less than an hour but can not provide continuous measurements at a point. Satellites provide data on the regional scale variability of the spectral reflectances at horizontal resolutions from 25 m (Landsat Thematic Mapper) to 1 km (Advanced Very High Resolution Radiometer) but cloud free conditions are required. However, regional scale observations are desirable because they are directly comparable to the output from General Circulation Models (GCM) and they provide the link between the patch and continental scales. There is much data on surface-atmosphere exchange at the leaf and patch scales but little such data at regional and continental scales (Raupach et al., 1994; Wang and Barrett, 2003).

The terms microscale, mesoscale and macroscale will be used to group the scales and the heterogeneity being discussed (Raupach and Finnigan, 1995). For typical daytime conditions during OASIS, these correspond to < 2 km, 2 km to 50 km and > 50 km respectively.

### 1.2.3 The Energy Balance and Available Energy

At the global scale, the Earth and its atmosphere form a closed system. Energy arrives in the form of shortwave radiation from the Sun and leaves in the form of reflected shortwave and emitted longwave radiation from the Earth' s surface and atmosphere. This simple balance hides great complexity.

At the hemispheric scale, the decrease in solar elevation with increasing latitude leads to a net gain of energy at the Equator and a net loss at the Poles. The weather and ocean currents of everyday experience are the resultant motions that seek to restore this imbalance by the poleward transport of sensible and latent heat. The motion of the atmosphere results in wind shear, the vertical increase in wind speed with height above the surface, in accordance with the no-slip condition at the surface. The consequence of this shear is turbulence, enhanced or suppressed by buoyancy forces, and the end point of turbulence is dissipation by viscous forces. Our area of interest, the turbulent exchange of heat, moisture and CO<sub>2</sub> between the surface and the atmosphere, occurs against the backdrop of, and as part of, the much larger exchange of the global energy budget.

At the patch and regional scales, the surface energy balance (SEB) can be written as (Oke, 1987):

$$F_A = F_N - F_G = F_H + F_E \quad 1.2$$

Here  $F_A$  is the available energy,  $F_N = S_{\downarrow} - S_{\uparrow} + L_{\downarrow} - L_{\uparrow}$  is the net radiation at the surface and  $S_{\downarrow}$ ,  $S_{\uparrow}$ ,  $L_{\downarrow}$  and  $L_{\uparrow}$  are the incoming and outgoing short and longwave radiations respectively.  $F_G$  is the conduction of heat into the ground,  $F_H$  is the sensible heat to the atmosphere and  $F_E$  is the latent heat transfer as water vapour. The change in energy storage at the surface and the energy absorbed during photosynthesis in the vegetation canopy, neither of which exceeds a few percent of  $F_N$  (Oke, 1987), have been neglected in writing Equation 1.2 and are not considered in this thesis.

Equation 1.2 is a powerful constraint on  $F_H$  and  $F_E$  but its apparent simplicity is deceptive. First, it combines three distinct forms of energy transport, radiative ( $F_N$ ),

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conductive ( $F_G$ ) and convective ( $F_H$  and  $F_E$ ). Second, the terms are usually assumed to represent the vertical components only of the associated fluxes, in particular  $F_H$  and  $F_E$  are assumed to be the vertical components of the turbulent fluxes. Advection is not routinely considered when evaluating Equation 1.2 (Lee, 1998; Finnigan, 1999; Lee, 1999; Paw U et al., 2000). Third, the components of the SEB, and the instruments used to measure them, do not exhibit the same behaviour with frequency. In particular, the equality expressed in Equation 1.2 requires the assumption that the period over which the measurements are averaged coincides with a frequency at which none of the components has significant power, that is, it lies within a spectral gap (Sakai et al., 2001; Kanada et al., 2004). Fourth, each measurement is representative of a different source area at the surface (Schmid, 1997). Fifth, extraction of the vertical turbulent components of  $F_H$  and  $F_E$  involves data processing steps, such as coordinate rotation and trend removal, that may result in the loss of low frequency contributions (Finnigan et al., 2003).

These issues contribute to the difficulty of obtaining closure of Equation 1.2 when using experimental data (Mahrt, 1998; Massman and Lee, 2002; Kanada et al., 2004). This has been observed repeatedly in studies using eddy covariance measurements of the turbulent fluxes where  $F_H + F_E$  is routinely less than  $F_N - F_G$  by up to 30% of the available energy (Sakai et al., 2001). This has a number of implications. At a fundamental level, it casts doubt on our understanding of the dynamics of surface-atmosphere interaction and our ability to accurately quantify the processes responsible. It also suggests that some processes hitherto regarded as unimportant are, in fact, significant. At a practical level, it limits the accuracy of model validation studies and may lead to the under-estimation of water loss and CO<sub>2</sub> uptake by vegetation if the eddy covariance measurement of these fluxes is in error. Methods have been proposed for dealing with this bias (Twine et al., 2000) but they lack a rigorous physical basis.

This bias, or systematic error, is one of two aspects of the SEB closure problem. The second is the deviation of results from individual averaging periods about any overall bias, that is, the scatter in plots of  $F_H + F_E$  versus  $F_N - F_G$ . This aspect has received much less attention in the literature even though the scatter, as a percentage of the

available energy, is often much larger than the overall bias. One possible reason for the observed scatter is random error in the measurements of the turbulent fluxes (Mahrt, 1998) and one of the major contributors to random errors in flux measurements is non-stationary conditions. Averaging measurements of the SEB components over longer periods can reduce the effect of non-stationary conditions but while this reduces the deviation between  $F_H + F_E$  and  $F_N - F_G$ , it does not eliminate it. For example, the standard error in the comparison of  $F_H + F_E$  and  $F_N - F_G$  at one of the main OASIS ground-based sites (Wagga pasture, see Chapter Two) is  $65 \text{ W m}^{-2}$  for hourly data and this reduces to  $37 \text{ W m}^{-2}$  for daily averages.

The importance of systematic and random errors in the SEB increases substantially when plant physiological quantities such as canopy conductance (Thom, 1975) are inferred from micrometeorological measurements. These inferences are often made through inversion of models such as the Penman-Monteith equation (Thom, 1975). Systematic errors in the input data then translate into bias in the inferred quantity and random errors in the input data can produce spurious estimates. Both of these processes are exacerbated if the model equations are non-linear. It is worthwhile noting that these problems are largely hidden when the turbulent fluxes are estimated using the Bowen ratio technique since this method forces closure of the SEB for each measurement period. Eddy covariance may well be the better technique for measuring  $F_H$  and  $F_E$ , not only because it involves fewer assumptions but also because it forces us to recognise the imperfection of our measurements.

Moving to the leaf scale, the energy balance for a leaf can be written as:

$$F_{N,leaf} = F_{H,leaf} + F_{E,leaf} \quad 1.3$$

The storage of energy and the energy used by photosynthesis have again been neglected and the ground storage term is no longer necessary. However, the situation is at least as complex as that for the SEB. The net radiation term,  $F_{N,leaf}$ , must take into account the orientation of the leaf with respect to the Sun and the attenuation of light within the vegetation canopy.  $F_{H,leaf}$  and  $F_{E,leaf}$  still represent the loss of energy from the control surface, in this case the leaf, to the air via sensible and latent heat but these exchanges occur within the complex flows encountered in

vegetation canopies (Kaimal and Finnigan, 1994). Despite these complications, the great utility of Equation 1.3 lies in the role it plays in the derivation of the Penman-Monteith equation (Thom, 1975; Kaimal and Finnigan, 1994), perhaps the most widely used model of evapotranspiration.

### 1.2.4 Evapotranspiration

Evaporation is the direct loss of water from a wet surface. In the context of the surface-atmosphere exchanges considered here, the relevant surfaces are the soil and any external plant surfaces such as leaves and stems that may be wet after precipitation.

Transpiration is the loss of water by vegetation through microscopic pores on the leaf surface called stomata. Plants grow by photosynthesis, the photochemical transformation of carbon dioxide ( $\text{CO}_2$ ) and water ( $\text{H}_2\text{O}$ ) to carbohydrates (plant material, sugars) and oxygen ( $\text{O}_2$ ) that occurs within the leaf (Oke, 1987). Water is absorbed from the soil by the plant root system and supplied to the leaf interior by the xylem.  $\text{CO}_2$  enters the leaf interior by diffusing through the stomata but, since the stomata must be open for this process to occur, water vapour diffuses out and is lost to the atmosphere. By opening and closing the stomata in response to environmental stimuli, plants are able to exert a large degree of control over the water lost in exchange for the  $\text{CO}_2$  gained.

Evapotranspiration is the term used to describe the total exchange of water between the surface and the atmosphere and consists of two components, evaporation from the soil and transpiration from the vegetation. In meteorology, evapotranspiration is quantified in terms of the latent heat flux ( $F_E$ ), the amount of energy required to evaporate the water lost by the surface, but in hydrology, it is usual to quantify evapotranspiration as an evaporation rate ( $E$ ) with the units of mass per unit area per unit time.

Evapotranspiration has an importance beyond its role in the exchange of water between the surface and the atmosphere (Pielke et al., 1998). It is the common term in the surface energy balance and the hydrological balance (Oke, 1987):

$$p = E + \Delta r + \Delta S \quad 1.4$$

where  $p$  is precipitation,  $\Delta r$  is the net runoff,  $\Delta S$  is the net change in soil moisture and  $E$  is the evaporation. As the common term, it directly links the energy and water cycles of the Earth-atmosphere system and provides common ground between the disciplines of meteorology and hydrology (Raupach and Finnigan, 1995). Transpiration also links the carbon and water cycles through the role of water in photosynthesis and the fact that both transpiration and assimilation are regulated by gaseous diffusion through the plant stomata.

In the simplest case, evaporation is driven by the available energy and modulated by the surface wetness, itself determined by the recent history of precipitation and evapotranspiration. At this simple level, in mid-latitude temperate areas, evaporation is primarily controlled by the energy input to the surface, essentially incoming shortwave radiation and albedo ( $\alpha = S_{\uparrow}/S_{\downarrow}$ ), and the wetness of the surface. The implication is that accurate prediction of the time history of evapotranspiration, say as one of the variables in a GCM, requires accurate prediction of cloud cover, since this is the dominant modulator of  $S_{\downarrow}$  after the diurnal cycle, and rainfall. Accurate cloud cover and rainfall predictions are still challenging for current general circulation models (McAvaney et al., 2001).

The available energy and the soil moisture also determine transpiration, with the additional control of stomatal function. Stomatal opening responds to several environmental conditions including the flux of photosynthetically absorbed radiation ( $F_{PAR}$ ), the saturation deficit ( $D = q^*(T_{leaf}) - q$  where  $q^*(T_{leaf})$  is the saturation specific humidity at the leaf temperature and  $q$  is the ambient specific humidity), the leaf temperature  $T_{leaf}$  and the ambient CO<sub>2</sub> concentration  $C$  (Oke, 1987). Stomata close when there is insufficient light, soil moisture or when the rate of water loss from the leaf interior becomes too great. Stomatal opening and closing has a profound effect on the energy balance at the leaf scale but the many feedback mechanisms stimulated by this change progressively reduce the effect as the scale increases (McNaughton and Jarvis, 1991). Some of these feedback mechanisms are discussed in Section 1.2.7.

The different components of the soil-vegetation-atmosphere continuum play different roles in water vapour exchange between the surface and the atmosphere. Moist soil and vegetation are both sources of water vapour. Their relative contributions to the total evapotranspiration depend primarily on the fractional vegetation cover, the leaf area per unit surface area (leaf area index,  $L_{ai}$ ) and the soil moisture profile from the surface through the root zone. In contrast, the daytime boundary layer is usually a sink for water vapour and this is maintained by the diurnal temperature cycle and the entrainment of dry air from the free troposphere as the ABL grows. The configuration of a surface source and an ABL sink results in a single direction for the transport of water vapour from the surface to the free troposphere above the ABL (Cleugh et al., 2004).

### 1.2.5 Sensible Heat

The other turbulent flux in the SEB is the sensible heat flux,  $F_H$ . This term describes the exchange of heat between the surface of the Earth and the ABL.

Shortwave radiation from the Sun warms the surface during the day. In the absence of strong advection, the surface temperature soon becomes greater than the air temperature, the air in contact with the surface is warmed by conduction and this air, now less dense than its surroundings, lifts away from the surface, transporting heat into the ABL by convection. The sensible heat flux is defined as positive under these conditions, when heat is transported away from the surface. The reverse process occurs at night when the emission of longwave radiation cools the surface and, by conduction, the air in contact with it. The resultant density gradient tends to inhibit vertical exchange but the shear forces resulting from the increase in wind speed with height can still generate turbulence, displacing the cooler, more dense air at the surface with warmer, less dense air from aloft. This results in a transport of heat from the ABL into the surface and the sensible heat flux is defined as negative. The partitioning of the available energy into latent (evapotranspiration) and sensible heat fluxes determines the magnitude of these transports and, in the special case of warm air flowing over well watered vegetation, may even influence the direction of the transport (Thom, 1975). The factors controlling the partition of available energy

include the surface type, the state of the vegetation (if present), the soil moisture and the meteorological conditions.

The flux of sensible heat into or away from the surface has two important consequences for the ABL. Firstly, the flux of heat into the daytime ABL results in a steady increase in the air temperature from sunrise to mid-afternoon. Secondly, it introduces buoyancy forces by virtue of the relationship between density and temperature and these have a profound affect on the structure of the ABL.

During the day, when  $F_H$  tends to be positive, buoyancy forces enhance or even dominate the shear production of turbulence. Buoyancy forces act to suppress the turbulence generated by shear forces when  $F_H$  is negative. In this way,  $F_H$  is a fundamental indicator of the stability of the ABL, a role that is formalised through the stability parameter  $z/L$  (see Equation 1.1), the ratio of the rates of turbulence production by shear and buoyancy forces (Kaimal and Finnigan, 1994).

The buoyancy forces resulting from the flux of sensible heat away from the surface produce organised vertical motions that extend to the top of the ABL. These act to mix air throughout the depth of the ABL on time scales of  $10^2$  to  $10^3$  seconds (Raupach and Finnigan, 1995). These times are short compared to the diurnal cycle and enable the ABL to reach a state of quasi-stationarity over homogeneous surfaces. The same vertical motions are also responsible for the growth of the ABL because they overshoot the inversion at the top of the boundary layer and then entrain free troposphere air into the boundary layer as they collapse back to their buoyancy height. The entrainment of relatively warm and dry tropospheric air is an important mechanism in determining the temperature, water vapour and  $\text{CO}_2$  concentrations of the mixed layer and through these, the surface fluxes of heat, water vapour and  $\text{CO}_2$  (Raupach, 1998).

As with water vapour, different components of the soil-vegetation-atmosphere system play different roles in the exchange of heat between the surface and atmosphere. The vegetation and the soil are again sources and so, in the case of heat, is the free troposphere. The fact that the daytime ABL is bounded, top and bottom, by sources of heat results in fluxes of opposite signs at the surface and at the top of the mixed layer. This is in contrast to the case for water vapour where the free

troposphere is a sink and the fluxes at the top and bottom of the ABL are in the same direction (Cleugh et al., 2004).

### 1.2.6 CO<sub>2</sub> Flux

Plant growth requires the assimilation of carbon dioxide during gross photosynthesis and the release during respiration of CO<sub>2</sub> by the metabolic processes powering that growth. Net photosynthesis is the difference between assimilation and respiration by the plant and corresponds to the dry matter gain by the plant. Oke (1987) gives a brief description of the chemical pathways of these processes.

Gross photosynthesis, also known as Gross Primary Productivity (*GPP*), requires solar radiation with a wavelength between 0.40 and 0.70  $\mu\text{m}$ , photosynthetically active radiation ( $F_{PAR}$ ). This restricts photosynthesis to daytime conditions but respiration occurs during the day (light respiration) and at night (dark respiration). Assimilation is also restricted to the green parts of the plant whereas respiration occurs from the above and below ground parts of the plant (autotrophic respiration) and from soil organisms and decomposing organic matter (heterotrophic respiration) (Kirschbaum et al., 2001). The relative contribution of these processes to the overall carbon budget for the plant depends on plant vigour, environmental factors and averaging period. At the global scale, autotrophic and heterotrophic respiration are often assumed to be approximately 50% and 40% of gross photosynthesis respectively (Steffan et al., 2000; Gifford, 2001). At the leaf, canopy and regional scales, these contributions can vary greatly so that an individual ecosystem may be either a source or a sink of CO<sub>2</sub> at any given time. This variability is further enhanced in some biomes by episodic loss due to disturbances such as land use change, fire and harvesting.

*GPP*, autotrophic respiration, heterotrophic respiration and loss due to disturbance can be arithmetically combined to give important measures of biome productivity. These are of use when estimating yields in agriculture and horticulture or when investigating the carbon cycle at large scales and help to demonstrate the importance of regional scale estimates of the CO<sub>2</sub> flux. Net Primary Production (*NPP*) is the difference between *GPP* and autotrophic respiration ( $R_a$ ):

$$NPP = GPP - R_a \quad 1.5$$

$NPP$  is important because it is related to biome growth in response to climatic and nutrient variables and can be estimated from remotely sensed quantities such as absorbed  $F_{PAR}$  (Field et al., 1995). The difference between  $NPP$  and heterotrophic respiration ( $R_h$ ) is the Net Ecosystem Productivity ( $NEP$ ):

$$NEP = NPP - R_h \quad 1.6$$

$NEP$  is important because it can be estimated from micrometeorological measurements (Lee, 1998; Baldocchi et al., 2000) and this realisation has stimulated the recent proliferation of long term observations of the SEB and  $CO_2$  flux at sites across the globe (Baldocchi et al., 2001a). Finally, the difference between  $NEP$  and  $CO_2$  loss due to disturbance,  $L_d$  is the Net Biome Productivity ( $NBP$ ):

$$NBP = NEP - L_d \quad 1.7$$

$NBP$  is important because it is the appropriate measure for long term, decadal or greater, changes in terrestrial carbon stores.

Micrometeorological measurements of surface-atmosphere exchange have an important place in quantifying  $NPP$  and  $NBP$ . Measurements of the  $CO_2$  flux combined with estimates of the  $CO_2$  storage and advection provide direct measurements of  $NEP$  at canopy and regional scales. A model of  $R_h$  can be used with the measurements of  $NEP$  to estimate  $NPP$  and these estimates can be compared with  $NPP$  derived from models, including those that use remotely sensed data. Further, either models or observations of  $L_d$  can be used with measured  $NEP$  to estimate  $NBP$  which, if available at continental and global scales, can be compared with estimates based on the accumulation of  $CO_2$  in the atmosphere.

As with water vapour and sensible heat, it is useful to examine the sources and sinks of  $CO_2$  in the ABL. Plants act as a sink for  $CO_2$  during the day provided sufficient soil water is available but they become a source of  $CO_2$  at night when photosynthesis is halted and respiration continues. The soil is a source of  $CO_2$  during the hours of both daylight and darkness. This is in contrast to the case for water vapour and

sensible heat where the plant canopy and the soil are both sources during the day and sinks at night. The free troposphere above the ABL acts as a source during the day as CO<sub>2</sub>-rich air is entrained into the ABL to offset the drawdown due to photosynthesis. The net transport of CO<sub>2</sub> during the day is then downward from the free troposphere to the surface, the reverse direction to the water vapour transport (Cleugh et al., 2004).

### 1.2.7 Scale Transitions

Surface-atmosphere exchange in the ABL occurs at leaf, canopy and regional scales. Those processes occurring at the leaf scale are directly accessible by observations made with porometers, leaf and soil chambers. Processes at the canopy scale are directly accessible by micrometeorological techniques such as eddy covariance and flux-profile methods. There is no corresponding measurement technique that gives direct access to exchange at regional and larger scales and these must be inferred from combinations of measurements and models or extrapolated from measurements made at smaller scales. The problems of scale transition arise when we attempt to apply the knowledge gained at one scale to another scale. For example, there is a wealth of knowledge about gas exchange at the leaf scale but much less is known about the fluxes at the canopy and regional scales. To overcome these gaps, knowledge of leaf scale processes is often used to provide a framework, if not a methodology, for investigating the processes at canopy and regional scales.

The treatment of evapotranspiration at leaf and canopy scales provides a good example of the dangers and difficulties of a simple approach to the transition between scales. The Penman-Monteith equation (Thom, 1975) is frequently used to model the exchange of water vapour at the leaf scale, between a leaf and the surrounding air, and at the canopy scale, between a canopy and the surface layer of the ABL. The appeal of using the same equation to describe evapotranspiration at different scales is twofold. Firstly, it adheres to the principle of the conservation of complexity (Raupach and Finnigan, 1995). Secondly, it allows the various terms to be interpreted in an analogous fashion. For example, there must be energy available to drive evaporation, water vapour must diffuse away from the source across a boundary layer and there is some physiological control of the process, stomatal

conductance  $g_s$  at the leaf scale and surface conductance  $G_s$  at the canopy scale. However the second point hides the subtleties of the first. While some processes retain their significance at different scales, others become insignificant and new processes become significant as the scale changes. In this case, retaining the same equation form across different scales requires that the changing roles of various processes must be reflected in the definitions of the model parameters.

McNaughton and Jarvis (1991) present an elegant description of this by using control theory to examine the feedback mechanisms that control transpiration at leaf and canopy scales. Their analysis shows that the number of negative feedback mechanisms increases when moving from the leaf to the canopy scale, increases again when going from the canopy to the regional scale and that this decreases the sensitivity of regional scale evapotranspiration to stomatal control. Raupach (1998) integrates a coupled assimilation-stomatal conductance model from leaf to canopy scale and uses this with a CBL slab model to examine the role of four feedback mechanisms at the canopy scale. He concludes that radiative feedback is not significant over rough surfaces and that the stomatal closure induced by high surface temperatures and large saturation deficits is mitigated by the effect of increasing instability on the aerodynamic conductance. Albertson et al. (2001) use a large eddy simulation (LES) model and a coupled assimilation-conductance model to investigate the controls on the fluxes of heat, water vapour and  $\text{CO}_2$  at the patch ( $\sim 10^2$  m) scale over a heterogeneous forest. They conclude that there is a quasi-linear relationship between the fluxes and  $L_{ai}$  and that several negative feedbacks act to minimise the variation in the water-use efficiency ( $F_C/F_E$ ) as  $L_{ai}$  varies. Anderson et al. (2003) discuss some aspects of feedback mechanisms at the regional scale and show how these can be encapsulated in models for scaling fluxes at the canopy level up to regions and for the reverse process of disaggregation. Current knowledge on biosphere-atmosphere interaction and feedback at regional, continental and global scales is reviewed by Pielke et al. (1998). They conclude that changes in these interactions, that is, changes in the momentum, heat and mass fluxes, are as important as more traditional climate disturbances such as changes in

"atmospheric dynamics and composition, ocean circulation, ice sheet extent, and orbital perturbations".

To conclude this section, the main points can be summarised as follows. It would be helpful if knowledge of surface-atmosphere interaction gained at one scale could be used to inform investigations at other scales. In particular, it would be useful to retain the same model form at several scales to aid interpretation of the model results and dependencies. However, this simple approach is confounded because an increase in the scale at which land-atmosphere interaction is investigated brings with it an increase in complexity on two fronts. Firstly, the heterogeneity of the surface increases as the scale increases and methods must be found to correctly average surface properties over a changing surface. The move from leaf to canopy scale can be made by integration of an expression for the stomatal conductance to obtain expressions for the canopy conductance (Kelliher et al., 1995; Raupach, 1995). The move from canopy to regional scale can be made by adoption of an appropriate averaging scheme (McNaughton, 1994; Raupach and Finnigan, 1995; Hu et al., 1999). Secondly, the number of controlling mechanisms increases as the scale increases and smaller scale processes must be parameterised or the small-scale model must be embedded in a larger scale model. Examples of this are the coupling of the Penman-Monteith equation with a CBL model to study regional evaporation (McNaughton and Spriggs, 1986) and the incorporation of soil-vegetation-atmosphere transport (SVAT) models into general circulation models (Avissar, 1995) to study global scale climate. Finally, most of the discussion on scale transition concerns the fluxes of heat and water vapour, both of which play a role in the thermodynamics of the ABL. This is not the case for  $\text{CO}_2$  and in general, the feedback mechanisms that control  $F_E$  will not be the same as those for  $F_C$  and for this reason, conclusions reached about the level of sophistication necessary to model  $F_E$  at various scales (McNaughton and Jarvis, 1991) may not apply to  $F_C$ .

### 1.2.8 Surface Properties

Both meteorological quantities and surface properties determine the fluxes of momentum, heat, water vapour and  $\text{CO}_2$ . This is evident in the Penman-Monteith

equation and the aerodynamic form of the CO<sub>2</sub> flux. These separate the fluxes into components due to the meteorology, such as gradients of  $q$  and CO<sub>2</sub> concentration  $C$ , available energy  $F_A$ , wind speed  $U$ , and those due to the surface such as roughness length  $z_0$  and stomatal conductance  $g_s$ . The temporal variation of the fluxes is dominated by the diurnal cycle in the meteorology whereas the properties of undisturbed surfaces change on longer time scales of weeks or more (Baldocchi et al., 2001b). Conversely, the spatial variation in fluxes over a heterogeneous surface is dominated by the spatial variation in surface properties (Mahrt et al., 1994; Ogunjemiyo et al., 1999; Lyons and Halldin, 2004) whereas meteorological quantities become horizontally uniform above the blending height (Mahrt, 2000). This suggests that most of the temporal variation in regional scale fluxes is contained in the meteorological forcing and that most of the spatial variation is contained in the surface properties.

Baldocchi et al. (2001b) examined a four-year time series of half-hourly observations of fluxes and mean meteorological quantities measured over a deciduous forest in North America. Their results show that spectra of  $F_E$  and  $F_C$  have significant peaks at semi-diurnal (12 hours), diurnal (24 hours) and synoptic (3 to 5 days) time scales, a pronounced spectral gap at quasi-monthly (20 to 30 days) scales and a broad peak at seasonal to annual scales. Cospectra and coherency spectra of air temperature ( $T_a$ ) and photosynthetically active radiation ( $F_{PAR}$ ) with  $F_C$  show peaks at semi-diurnal, diurnal, seasonal and annual time scales. In contrast, a spectrum of leaf area index shows little variance in  $L_{ai}$  at time scales shorter than 30 days. Baldocchi et al. (2001b) also compare spectra of measured and modelled  $F_C$  and show that the model is able to reproduce the time scales in the observations even when the surface properties (leaf area and photosynthetic capacity) are slowly varying (D. Baldocchi, 2004, pers. comm.).

Three characteristics are required of a surface property if it is to be useful in modelling regional scale fluxes. First, it should be related to vegetation type, condition and fractional cover. Secondly, it should have a diurnal trend that is predictable from basic meteorological quantities. This includes the special case of

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no diurnal trend. Thirdly, it should be insensitive to synoptic conditions although it may respond to seasonal changes in soil moisture, air temperature and plant physiology. These characteristics also mean that the surface property can be estimated from infrequent observations such as those available from research aircraft and satellites.

Four surface properties are considered in this thesis. Three of these are simple ratios of the fluxes of available energy, heat, water vapour and CO<sub>2</sub>: the Bowen ratio  $\beta = F_H / F_E$ , the evaporative fraction  $\alpha_E = F_E / F_A$  and the water-use efficiency  $W_{UE} = \lambda F_C / F_E$ . The fourth is a measure of the stomatal conductance of the underlying vegetation, in this case the maximum stomatal conductance  $g_{sx}$  (Kelliher et al., 1995). The simple ratios can be calculated directly from the measured fluxes. The maximum stomatal conductance is estimated from observations of the fluxes by coupling the Penman-Monteith equation to a simple model of canopy conductance.

### 1.3 Thesis Hypothesis

The following hypothesis is proposed:

That regional scale fluxes of heat, water vapour and carbon dioxide can be calculated from time-varying meteorology measured at a central location and spatially-varying surface properties inferred from remotely sensed data.

The method that ensues from this hypothesis does not follow the same path as the upscaling of observations from leaf to canopy scales, where averaging schemes that conserve the total flux can be used (McNaughton, 1994; Raupach, 1995). Rather, the extension to regional scales is achieved with a simple model in which bulk meteorological quantities measured at a central location provide the diurnal forcing and surface properties, either spatially-averaged or spatially-resolved, provide the variability of the fluxes across the landscape. Direct measurements of spatially-averaged surface properties are available from aircraft observations and it will be shown that spatially-resolved surface properties can be inferred from remotely sensed data.

The hypothesis is tested in four steps. First, aircraft and ground-based observations during the 1995 OASIS experiment are compared in order to establish their compatibility, a necessary step before these data can be integrated. Second, the diurnal trends in, and synoptic sensitivity of, four surface properties are examined in order to evaluate their potential to describe the spatial variability in the surface fluxes. Third, the surface properties are related to remotely sensed data and these relationships are used to interpolate the surface properties across an area of 130 by 50 km. Finally, regional scale fluxes of sensible heat, latent heat and CO<sub>2</sub> are calculated using the interpolated surface properties and meteorology measured at a single location and these fluxes are compared to the available observations and to estimates from two other methods.

### 1.4 Thesis Outline

This thesis consists of eight chapters, including this introduction. It starts with a discussion of the data to be used before developing and validating two methods for estimating regional scale fluxes of heat, water vapour and CO<sub>2</sub>. The hypothesis is then tested using results from the methods.

Chapter Two describes the OASIS experiments with emphasis on the 1995 observing period. An overview of the OASIS experiments is given first, followed by descriptions of the location, instrumentation and data processing of the ground-based sites, a description of the aircraft flight programme and details of the remote sensing data used in this work. The chapter finishes with a discussion of the general meteorology of the 1995 OASIS experiment and some concluding remarks.

Chapter Three describes the aircraft instrumentation used during the 1995 OASIS experiment and the calibration of these instruments before, during and after the 1995 experiment. The calibration of the aircraft instrumentation is separated into two parts. Static calibration describes the techniques used to obtain absolute calibrations of the pressure, temperature, water vapour, CO<sub>2</sub> and radiation sensors with the instruments removed from the aircraft or with the aircraft at rest. Dynamic calibration refers to the techniques used to obtain the corrections to the static calibrations to account for the motion of the aircraft through the air. A comprehensive model for calculating the aircraft true airspeed and the angles of attack and sideslip is adopted, applied to the results from a dedicated calibration flight and optimised using data collected during the 1995 OASIS experiment. The chapter ends with a description of the known instrumentation problems.

A detailed comparison of aircraft and ground-based observations was conducted as part of the analysis of data from the 1995 experiment and the results of this are presented in Chapter Four. The chapter begins with a brief explanation of data processing techniques applied to the aircraft data and a discussion of random errors in measurements of variance and covariance. Aircraft observations from nine low-level flights are compared to ground-based observations. These flights were designed to minimise the systematic errors in comparisons between aircraft and

ground-based measurements of means, variances and covariances. Aircraft and ground-based observations of the fluxes are also compared for all times when the aircraft was in the vicinity of a ground-based site during the 1995 experiment. The results are discussed with particular attention to systematic errors arising from flux divergence, sampling limitations and surface heterogeneity. The work presented in this chapter is an extension of that presented in Isaac et al. (2004a).

Four surface properties are examined in Chapter Five. Two describe the partitioning of energy at the surface, one describes the maximum stomatal conductance achievable by leaves at the top of a well-watered canopy and the fourth is the ratio of CO<sub>2</sub> flux to evapotranspiration. The surface properties are introduced, defined and the model for estimating  $g_{sx}$  from observations of  $S_{\downarrow}$ ,  $F_A$ ,  $F_E$ ,  $T_a$  and  $D$  is described. The sensitivity of the estimated surface properties to random and systematic errors in the surface energy budget components is discussed and the averaging techniques used to reduce this sensitivity are described. The utility of the surface properties for estimating regional scale fluxes is then examined by investigating their diurnal, daily and spatial variability.

Chapter Six relates the surface properties to a remotely sensed quantity, the Normalised Difference Vegetation Index ( $NDVI$ ), using a model of the source-area weight function. The chapter begins with a description of the remote sensing data and the calculation of  $NDVI$  and a description of the source-area model and the calculation of the source-area weighted  $NDVI$  follows. The source-area weight model is applied to the remote sensing data using both ground-based and aircraft data and the relationship between the source-area weighted  $NDVI$  and the surface properties is explored. This exploration is motivated by the belief that remotely sensed quantities such as  $NDVI$  will be better correlated with surface properties than with the surface fluxes themselves. The relationships between  $NDVI$  and the surface properties are then used to extend the observations across an area of 130 km by 50 km.

The surface properties are used to calculate the regional-scale fluxes of water vapour, sensible heat and carbon dioxide for the OASIS domain and the results of these analyses are compared to estimates from other methods in Chapter Seven. The

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models for estimating regional scale fluxes are presented and the spatial variability of meteorological quantities is investigated. In particular, the extent to which measurements at a single point can be applied to a 130 km by 50 km region is investigated, by comparing the site-to-site correlation of the fluxes and the bulk meteorological quantities. Daily averaged fluxes of latent heat, sensible heat and CO<sub>2</sub> estimated using the surface properties are compared to the available observations for a 10 km by 10 km area, along a 96 km transect and for a 130 km by 50 km region. At the regional scale, the results are also compared to those from CBL budget methods and a coupled mesoscale-SVAT model.

The conclusions of the thesis are presented in Chapter Eight.