Improved estimation of surface biophysical parameters through inversion of linear BRDF models

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Supervised by Dr. P. Lewis
Artist's impression of the NASA Terra platform, launched in December 1999 as part of long term efforts to monitor and understand global climatic and circulation processes (courtesy of NASA).

False colour representation of global land surface reflectance and sea surface temperature derived from instruments aboard the Terra platform (courtesy of NASA).
Abstract

An investigation is presented into the ability of linear kernel-driven models to adequately describe the surface bidirectional reflectance distribution function (BRDF) of vegetation. Such models were developed primarily for deriving albedo from limited angular samples of reflectance at moderate resolution (100s of m to km) and are based on semi-empirical approximations to more complex physically-based models. They assume that BRDF can be described by a linear combination of separate scattering 'shapes' (kernels), each of which is a function of purely geometric terms (viewing and illumination angles) only.

The assumptions underlying the linear kernel-driven models were tested using 3D geometric canopy structural models allied to a description of the radiometric scattering behaviour within the 3D canopy. This is the first time the properties of the models have been explicitly tested in this manner. The assumption that canopy reflectance can be represented as a linear combination of volumetric and geometric-optic (GO) scattering terms appears to be well founded. The kernels perform less well when the canopy departs too far (structurally or radiometrically) from the assumptions made in the model formulation. It is shown that the volumetric and GO kernels are not always capable of separating the components of canopy reflectance and that there can be coupling between the kernels. It is also demonstrated that the model parameters are not purely geometric as intended and that they contain biophysical information (related to leaf area and leaf reflectance). However, this information may require ancillary data if it is to be extracted from the model parameters.

A linear kernel-driven model of spectral reflectance is proposed which would allow interpolation (and extrapolation) of narrowband spectral samples of reflectance across the solar spectrum. Results suggest that this approach is very effective and can complement the angular kernels, allowing a full spectral, directional kernel-driven description of canopy reflectance. This is likely to prove extremely useful for deriving broadband albedo and for separating the spectral components of soil and vegetation scattering for studies of canopy-atmosphere transfer and productivity.
Acknowledgements

Firstly, I want to thank my supervisor, Lewis. He has provided far more inspiration and help than I probably deserve. He taught me that it can actually be fascinating watching (and understanding) grass grow. I owe my interest and continued development in plant modelling (and much else) to him. I would also like to thank colleagues such as Crystal Schaaf and the BU MODIS team, Jean-Louis Roujean, Charlie Walthall and in particular Mike Barnsley, for influence and guidance over the last few years. Thanks also go to colleagues within the Department of Geography at UCL for stimulating conversation over the years. I owe a debt of gratitude I can never repay to my Mum and Dad for always supporting me and making me realise what an incredible place the world is. Finally, above all else, I must thank Helen. For supporting me (financially and emotionally), for getting me through the bad and for sharing the good. Without you, it wouldn't be worth it. Helen, this is for you (maybe one day you'll read it!).

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<th>Description</th>
</tr>
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<tbody>
<tr>
<td>$A_{G,C,Z,T}$</td>
<td>Areal proportions of illuminated ground and crown, and shadowed ground and crown</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Albedo</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Volumetric component of canopy scattering</td>
</tr>
<tr>
<td>$\beta$</td>
<td>GO component of canopy scattering</td>
</tr>
<tr>
<td>$C$</td>
<td>Canopy clumping factor</td>
</tr>
<tr>
<td>$E$</td>
<td>Irradiance arriving at the surface</td>
</tr>
<tr>
<td>$F_{\downarrow}$</td>
<td>Downwelling (total) flux</td>
</tr>
<tr>
<td>$F_{\uparrow}$</td>
<td>Upwelling (total) flux</td>
</tr>
<tr>
<td>$f_{iso}, f_{vol}, f_{GO}$</td>
<td>Isotropic, volumetric and GO linear model parameters</td>
</tr>
<tr>
<td>$G(\Omega)$</td>
<td>Leaf projection function in viewing (or illumination) direction</td>
</tr>
<tr>
<td>$g(\Omega)$</td>
<td>Angular distribution of leaf normals</td>
</tr>
<tr>
<td>$\Gamma(\Omega \rightarrow \Omega)$</td>
<td>Leaf scattering phase function</td>
</tr>
<tr>
<td>$H$</td>
<td>Sensible heat flux</td>
</tr>
<tr>
<td>$I_{\downarrow}$</td>
<td>Downwelling diffuse flux</td>
</tr>
<tr>
<td>$I_{\uparrow}$</td>
<td>Upwelling diffuse flux</td>
</tr>
<tr>
<td>$k_{iso}, k_{vol}, k_{GO}$</td>
<td>Isotropic, volumetric and GO linear model kernels</td>
</tr>
<tr>
<td>$LE$</td>
<td>Latent heat flux</td>
</tr>
<tr>
<td>$L_e$</td>
<td>Radiance exitant from the surface</td>
</tr>
<tr>
<td>$L_{\downarrow}$</td>
<td>Downwelling radiance</td>
</tr>
<tr>
<td>$L_{\uparrow}$</td>
<td>Upwelling radiance</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Wavelength</td>
</tr>
<tr>
<td>$\mu, \mu'$</td>
<td>Cosine of view, illumination zenith angles</td>
</tr>
</tbody>
</table>
\( Q(\Omega' \rightarrow \Omega, z) \) Joint gap probability
\( \Omega(\theta_v, \phi_v) \) or \( \Omega \) Viewing vector (solid angle)
\( \Omega(\theta_i, \phi_i) \) or \( \Omega' \) Illumination vector (solid angle)
\( R_n \) Net radiation
\( \rho \) Reflectance
\( \overline{\rho}(\lambda, \Omega, \Omega') \) Spectral directional hemispherical reflectance
\( = \rho(\lambda) \) Spectral bihemispherical reflectance
\( \sigma_c \) Extinction coefficient of the canopy medium
\( \sigma_s \) Differential scattering coefficient of canopy medium
\( \tau \) Transmittance (in canopy) or optical depth (in atmosphere)
\( \theta_i, \phi_i \) Illumination zenith and azimuth angles
\( \theta_v, \phi_v \) View zenith and azimuth angles
\( w \) Weighting value
\( \omega \) Single scattering albedo
\( \zeta \) Phase angle of scattering
\( Z_o \) Surface roughness length
\( z \) Depth/height within canopy

**Acronyms/Abbreviations**

Each acronym/abbreviation is explained in the text when it is first introduced.

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Definition</th>
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<tbody>
<tr>
<td>ADEOS</td>
<td>Advanced Earth Observing System</td>
</tr>
<tr>
<td>AERONET</td>
<td>Aerosol Robotic Network</td>
</tr>
<tr>
<td>AIC</td>
<td>Akaike information criteria</td>
</tr>
<tr>
<td>AMBRALS</td>
<td>Algorithm for MODIS bidirectional reflectance and albedo</td>
</tr>
<tr>
<td>ANN</td>
<td>Artificial neural network</td>
</tr>
<tr>
<td>ARARAT</td>
<td>Advanced Radiometric Ray Tracer</td>
</tr>
<tr>
<td>ARS</td>
<td>Airborne Research System</td>
</tr>
<tr>
<td>ASAS</td>
<td>Advanced Solid state Array Spectrometer</td>
</tr>
<tr>
<td>ASTER</td>
<td>Advanced Spaceborne and Thermal Emission and Reflection Radiometer</td>
</tr>
<tr>
<td>ATM</td>
<td>Airborne Thematic Mapper</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>-------------</td>
</tr>
<tr>
<td>ATSR</td>
<td>Along Track Scanning Radiometer</td>
</tr>
<tr>
<td>AVHRR</td>
<td>Advanced Very High Resolution Radiometer</td>
</tr>
<tr>
<td>BPMS</td>
<td>Botanical Plant Modelling System</td>
</tr>
<tr>
<td>BRDF</td>
<td>Bidirectional reflectance distribution function</td>
</tr>
<tr>
<td>CASI</td>
<td>Compact Airborne Spectrographic Imager</td>
</tr>
<tr>
<td>CERES</td>
<td>Clouds and Earth’s Radiant Energy System</td>
</tr>
<tr>
<td>CHRIS</td>
<td>Compact High Resolution Imaging Spectrometer</td>
</tr>
<tr>
<td>CR</td>
<td>Canopy reflectance</td>
</tr>
<tr>
<td>CSAR</td>
<td>Coupled Surface-Atmosphere Reflectance</td>
</tr>
<tr>
<td>DART</td>
<td>Discrete Anisotropic Radiative Transfer</td>
</tr>
<tr>
<td>DEM</td>
<td>Digital elevation model</td>
</tr>
<tr>
<td>EGO</td>
<td>European Goniometric Observatory</td>
</tr>
<tr>
<td>ENVISAT</td>
<td>Environmental Satellite</td>
</tr>
<tr>
<td>EO</td>
<td>Earth observation</td>
</tr>
<tr>
<td>EOS</td>
<td>Earth Observing System</td>
</tr>
<tr>
<td>EPFS</td>
<td>Equipment Pool for Field Spectroscopy</td>
</tr>
<tr>
<td>ERS</td>
<td>European Remote Sensing Satellite</td>
</tr>
<tr>
<td>fAPAR</td>
<td>Fraction of absorbed photosynthetic radiation</td>
</tr>
<tr>
<td>FCC</td>
<td>False colour composite</td>
</tr>
<tr>
<td>GA</td>
<td>Genetic algorithm</td>
</tr>
<tr>
<td>GARP</td>
<td>Global Atmospheric Research Program</td>
</tr>
<tr>
<td>GCM</td>
<td>General/global circulation model</td>
</tr>
<tr>
<td>GO</td>
<td>Geometric optic</td>
</tr>
<tr>
<td>IFB</td>
<td>International Forum on BRDF</td>
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<tr>
<td>IFOV</td>
<td>Instantaneous field of view</td>
</tr>
<tr>
<td>IGBP</td>
<td>International Geosphere Biosphere Program</td>
</tr>
<tr>
<td>IPCC</td>
<td>International Panel on Climate Change</td>
</tr>
<tr>
<td>IWMM</td>
<td>International Workshop on Multiangle Modelling Methods</td>
</tr>
<tr>
<td>IR (NIR)</td>
<td>Infrared (near IR)</td>
</tr>
<tr>
<td>ISLSCP</td>
<td>International Satellite Land Surface Climatology Project</td>
</tr>
<tr>
<td>JRC</td>
<td>Joint Research Centre</td>
</tr>
<tr>
<td>KBS</td>
<td>Knowledge-based system</td>
</tr>
<tr>
<td>LAI</td>
<td>Leaf area index</td>
</tr>
<tr>
<td>LAD</td>
<td>Leaf angle distribution</td>
</tr>
<tr>
<td>LiDAR</td>
<td>Light detection and ranging</td>
</tr>
</tbody>
</table>
LOPEX Leaf Optical Properties Experiment
LSP Land surface process
LUT Look-up table
MISR Multi-angle Imaging Spectro-Radiometer
MODIS Moderate Resolution Imaging Spectroradiometer
MOPITT Measurement of Pollution in The Troposphere
MSG METEOSAT Second Generation
MTPE Mission To Planet Earth
MVA Multiple view angle
MVC Maximum value composite
NASA National Aeronautical and Space Agency
NDVI Normalised difference vegetation index
NERC Natural Environment Research Council
NOAA National Oceanic and Atmospheric Administration
NPOESS National Polar Orbiting Environmental Satellite System
NPP Net primary productivity
PCA Principal component analysis
POLDER Polarisation and Directionality of the Earth’s Surface
PROBA Project for On Board Autonomy
PSN (daily) net photosynthesis
RADAR Radio detection and ranging
RAMI Radiative Transfer Model Intercomparison
RMSE Root mean square error
RPV Rahman-Pinty-Verstraete
RT Radiative transfer
SAIL Scattering by arbitrarily inclined leaves
SOSA Successive orders of scattering approximation
SPOT Système Probatoire d’Observation de la Terra
SVAT Soil-vegetation-atmosphere transfer
SW Shortwave
TOA Top-of-atmosphere
TIR Thermal infrared
TM Thematic mapper
UNFCC United Nations Framework Convention on Climate Change
1 Introduction

1.1 Change and uncertainty in global climate

The development of remote sensing as a tool for better understanding the dynamics of biogeochemical processes controlling the Earth’s climate has been driven by a growing recognition of the need to determine human impact on the global environment (Global Atmospheric Research Program (GARP) report, 1975; Henderson-Sellers and Wilson, 1983; Sellers, 1994; Trenberth, 1995; Hall et al., 1995). This need has been exacerbated by the apparent increase in extreme climatic events of recent years such as the unusually long-lived and severe El Niño event of 1997-8, the subsequent droughts and fires in South East Asia and flooding in Central America in the latter part of 1998 (Webster and Curry, 1998). Such potentially catastrophic climate events have impacted virtually all aspects of human life around the globe: from minor regional climatic and ecosystem variability to life-threatening fires; the threat of sea-level rise inundating low-lying coastal regions (Schneider, 1999), to more indirect manifestations such as the instability of global economic and political conditions.

It is widely accepted that the increase in frequency of extreme climate events is related to changes in the overall global climate, and in particular, a gradual increase in global mean temperature over the past century (Intergovernmental Panel on Climate Change (IPCC), 1995a,b, 2001a,b, www[1.1]; International Geosphere Biosphere Program (IGBP), 1998). It is mooted that such changes may be the result of (or be exacerbated by) anthropogenic activities such as the burning of fossil fuels, intensified agriculture and urban development, amongst other activities (IPCC, 2001b; www[1.2]). Scientific uncertainty over the projected impact of anthropogenic impacts on global climate has also led to international political conflict, most notably over the US government’s refusal to ratify the United Nations Framework Convention on Climate Change (UNFCCC) ‘Kyoto protocol’ on planned reductions in CO₂ (www[1.3]). Uncertainty over cause and effect has polarised the scientific community in some respects (Musser, 2001) and a great deal of effort is now being expended to quantify this uncertainty (Visser et al., 2000; Wigley and Raper, 2001). Long term climate monitoring of global climate processes has been identified as key to this task. Other aspects of global change and the impact of human activity have raised more general issues, such as how best to sustainably exploit natural resources, how to monitor and/or prevent reductions in biodiversity and how to predict and adapt to potential changes in climate (www[1.4]). As
a result, many governments recognise the necessity of investing heavily in research aimed at developing a better understanding of both the underlying mechanisms and the actions of global climatic processes (Sellers, 1992).

The drive towards a better understanding of climate processes is exemplified by recent efforts such as NASA’s Earth Observing System (EOS) (formerly the Mission To Planet Earth (MTPE)). EOS is an ongoing series of experiments, instruments and projects, the stated aim of which is “...is to develop understanding of the total Earth system, and the effects of natural and human-induced changes on the global environment” (EOS press release, January 1998). As an indication of the seriousness with which such aims are being pursued, EOS was allocated a budget of $1.42 billion in the 1998 Congressional spending projections (ibid.). Other projects with similar aims are the Japanese Advanced Earth Observing System (ADEOS), with instruments such as POLDER (Polarisation and Directionality of the Earth’s Surface) on board, designed to measure land surface reflectance, polarisation, and atmospheric aerosol distributions (Deschamps et al., 1994; Leroy et al., 1996), and the next generation meteorological observation programme NPOESS (National Polar Orbiting Environmental Satellite System, www[1.5]).

In conjunction with developments in climate modelling such as rapid advances in computing speed and efficiency and sophistication of algorithms (Hack, 1995), Earth Observation (EO) has emerged as one of the most powerful tools for improving our understanding of the surface processes controlling global climate. Such processes operate over a huge range of spatial and temporal scales – from local and regional weather variations, to long-term warming and cooling trends of global climate. In order to detect perturbations in the global climate system (such as might be caused by anthropogenic increases in greenhouse gases like CO$_2$) methods of monitoring large (even global) areas over long time-scales are required (Charlson et al., 1992). The spatial coverage afforded by EO makes it particularly suited to such a task. Long-term temporal coverage will require successive generations of EO programmes. This has led to the inception of major international interdisciplinary projects such as the International Satellite Land Surface Climatology Project (ISLSCP) (Sellers, 1994), which aim to exploit the potential for timely, large-scale coverage offered by remotely sensed data (Sellers, 1992; IPCC 2001a,b).
1.2 Developments in Earth Observation

"[To] expand the observational foundation for climate studies to provide accurate, long-term data with expanded temporal and spatial coverage.... there is a need for long-term consistent data to support climate and environmental change investigations and projections."


A great deal of progress has been made in EO over the last thirty years. This has been driven largely by the realisation that the observation of global climate processes requires the type of spatial and temporal coverage only afforded by remote sensing. The current sophisticated, versatile and multi-purpose payloads exemplified by the NASA EOS programme (Running et al., 1994; Kaufman et al., 1998) represent a significant advance from the days of Landsat 1, a crude multispectral radiometer launched in 1972. A great deal of money and effort has been invested in developing remote sensing instruments to probe all aspects of global climate. This encompasses a wide range of processes including: the role of atmospheric aerosols and clouds in climate change (Charlson et al., 1992; Arking, 1991); ocean circulation and exchanges of latent and sensible heat with the atmosphere (Hsiung, 1985; Randall et al., 1992); carbon budget calculations (Schimel, 1995; IGBP, 1998; Wessman and Asner, 1998); biosphere-atmosphere transfer (Sellers et al., 1995); the influence of the cryosphere (Nolin and Stroeve, 1997); and absorption (and reflection/re-radiation) of incoming solar radiation at the Earth’s surface (Henderson-Sellers and Wilson, 1983; Dickinson, 1983, 1995).

The major obstacle to achieving more complete understanding of global climate processes has been identifying very gradual underlying long-term trends in global climate indicators beneath the highly variable short-term fluctuations of day-to-day weather patterns. The need for long-term, global data sets has led to an increased interest in the design and development of remote sensing platforms and methods specifically targeted at observing the Earth’s climatic processes. The NASA EOS program, with a number of planned missions, each carrying several complementary instruments, exemplifies the move towards a more comprehensive understanding of global climate processes through long-term integrated monitoring."
The EOS program is designed to monitor the interchanges of energy, moisture and carbon, land use, and ocean and atmospheric circulation for at least eighteen years. The EOS era began with the launch of the EOS-AM1 (*Terra*) platform in December 1999 (Kaufman et al., 1998. www[1.6]). The follow-up platform, EOS-PM1 (*Aqua*), designed to monitor hydrosphere and cryosphere processes, is due to be launched in 2002. To illustrate the comprehensive nature of EOS, the various instruments aboard the *Terra* platform are listed below:

- **ASTER** (Advanced Spaceborne and Thermal Emission and Reflection Radiometer) for monitoring local and regional processes such as surface temperature, energy balance and mapping of soils, geology and land cover change (Yamaguchi et al., 1998);

- **CERES** (Clouds and Earth’s Radiant Energy System) to determine the radiative forcing effect of Earth’s cloud cover and quantify the radiative budget (Wielicki et al., 1998);

- **MISR** (Multi-angle Imaging Spectro-Radiometer) a pointable instrument with nine look angles designed to observe the angular variations of scattering from the surface, atmospheric aerosols and clouds (Diner et al., 1998);

- **MODIS** (Moderate resolution Imaging Spectrometer) to provide comprehensive monitoring of land, ocean and atmosphere at moderate resolution, with high temporal coverage and capabilities to provide global estimates of land cover characteristics such as albedo (Justice et al., 1998).

- **MOPITT** (Measurement of Pollution in The Troposphere) for mapping atmospheric CO and CH₄ (Gilles et al., 1996).

Early results from Terra have already provided a remarkable look at the Earth’s climate processes and scientists are beginning to apply the data to some of the unanswered questions. Figure 1.1 is an example of reflectance data now being delivered by MODIS. This is one of 44 separate products delivered by MODIS now in their

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1 NASA is currently shifting the emphasis of future EO missions toward the ‘smaller, faster, cheaper’ model in order to reduce mission lead-in times and potential losses from failed missions.
advanced quality assurance phase before dissemination to the scientific community. These products represent a great improvement over data from sensors such as the National Oceanic and Atmospheric Administration (NOAA) Advanced Very High Resolution Radiometer (AVHRR). Greatly improved sensor technology and calibration combined with sophisticated processing have resulted in products usable by the wider community rather than just raw radiance data or simple empirical indices. The variety of long-term data from EOS, in conjunction with the Japanese Advanced Earth Observing System mission (www[1.7]) and European missions such as the Environmental Satellite (ENVISAT) (www[1.8]) and the European Remote Sensing satellites ERS-1 and 2 (www[1.9]), will enable a clearer understanding of the complex processes controlling Earth’s climate to be established. Data from a variety of such remote sensing platforms can also be combined to provide a synergistic view of the Earth’s climate processes.

1.3 Land surface processes

Land surfaces are particularly important in considering climate variability as they provide a lower boundary layer to the climate system (Dickinson, 1983; Graetz, 1991; Sellers, 1992; Dickinson, 1995). Ocean surfaces are generally more important in terms of the magnitude and mobility of stored heat energy but land surfaces tend to be far more spatially variable. As a result, land surface processes such as exchanges of moisture from the surface to the atmosphere, and reflection, absorption and re-radiation of incoming
solar radiation are far less spatially and temporally predictable than their ocean surface equivalents. Another major consideration is that human existence is almost exclusively dependent on the state of the land surface.

Earth observation has been deployed in many ways to improve understanding of land surface processes either by directly observing processes where possible or, in most cases, utilising observations made of surrogate (dependent) variables. One area where this is extremely important and of direct relevance to this thesis is the observation of surface biophysical parameters. Parameters such as total biomass, the fraction of absorbed photosynthetic radiation (fAPAR), transpiration rates, surface roughness ($Z_o$), and albedo provide linkages between biogeochemical processes such as nutrient availability, soil composition and the transfer of carbon and climatic drivers such as the fluxes of moisture and energy at the surface. These linkages take the form of near-surface atmospheric forcing, which in turn results in exchanges of water, radiation, and momentum between the surface and atmosphere (Sellers, 1995a). Consequently, much effort has been devoted to measuring and modelling land surface processes and their controlling biophysical parameters (Hall et al., 1995; Sellers, 1995b; Sellers et al., 1997).

1.3.1 Biophysical parameters and vegetation

In considering biophysical processes for inclusion into climate models, models of land surface processes (LSPs) have been developed (Dickinson, 1984; Sellers et al., 1986; Henderson-Sellers et al., 1993). A wide range of surface types (vegetation, ice/snow, desert) are considered when modelling land surface processes, each having their own regions of influence and importance. Vegetation is recognised as one of the most important cover types, both in terms of the linkage between biogeochemical processes and atmospheric circulation but also in terms of impact on human beings (Aber, 1995). For obvious reasons humans tend to favour vegetated areas over desert or snow and ice covered ones. In addition, processes controlling vegetation growth and development tend to have time-scales allowing them to strongly influence the atmospheric climate processes to which they link. For example, leaf-scale chemical processes such as photosynthesis have time-scales of a few seconds or less; evapotranspiration, CO$_2$, N$_2$ and nutrient fluxes vary over time-scales of days to weeks. These scales are similar to those over which
atmospheric energy transport processes such as turbulence, convection and radiation may act (Sellers, 1995a).

Vegetation is also an important factor in mediating interactions between the biogeophysical system and atmospheric circulation processes through the biophysical parameters mentioned above, such as fAPAR, $Z_o$ and albedo. An example of the influence of vegetation and the potential feedback on these surface-atmosphere interactions is illustrated in figure 1.2. This is the feedback cycle for surface roughness under hypothetical conditions of deforestation and/or desertification. Figure 1.2 emphasises that the energy exchanges between the surface and the atmosphere are heavily influenced by the quantity and activity of surface vegetation.

Figure 1.2 Potential positive and negative feedback loops resulting from large-scale change of surface albedo, $\alpha$. $R_n =$ net radiation, Wm$^{-2}$; $H =$ sensible heat flux (conduction to the air) Wm$^{-2}$; $LE =$ latent heat flux (through evaporation of moisture to the air) Wm$^{-2}$ (after Sellers, 1995).

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2 Albedo is not an intrinsic surface parameter due to its relationship with atmospheric state (see later).
The driver of all climate processes is incoming solar radiation. Consequently, understanding the fate of solar radiation arriving at the Earth's surface (through reflectance, absorption and/or re-radiation) is the key to understanding many of the major global climate processes. This thesis will concentrate on developments in measurement and modelling of incoming shortwave solar radiation interacting with vegetation. The emphasis is on shortwave radiation i.e. wavelengths from around 350nm up to 2500nm, as the vast majority of the radiant energy emitted from the sun lies in this wavelength range. Figure 1.3 shows the variation of incoming solar radiation with wavelength, in addition to the theoretical blackbody curve for a body at 5900° K (solar surface temperature). The energy distribution is sharply peaked around 0.55μm, which has driven the evolution of chlorophyll pigments in green vegetation which efficiently facilitate the conversion of incoming solar radiation into carbohydrates used in plant growth.

Figure 1.3 Solar irradiance at the top and bottom of the earth's atmosphere. Shaded areas indicate absorption by atmospheric gases (after Slater, 1980).
Remote sensing techniques have been applied in a number of areas in an effort to understand the processes affecting the Earth’s climate. One of the most important of these applications is that of shortwave energy budget studies: the study of the reflection and absorption of incoming shortwave (SW) i.e. visible and near-infrared (near IR, or NIR) solar radiation at the Earth’s surface, and its subsequent re-radiation into the atmosphere as thermal IR radiation. The role of surface reflectance in the Earth's radiation budget is illustrated schematically in figure 1.4. This demonstrates general mechanisms of solar interaction with the atmosphere and land surface.

![Diagram of solar radiation budget](image)

**Figure 1.4** The fate of incoming solar radiation at the Earth's surface (from [1.10]).

The absorption of solar energy at the Earth’s surface is the primary driving force behind all climatic processes (Dickinson, 1983). The amount of energy absorbed at the surface is determined by the surface albedo. Albedo ($\alpha$) is defined as the ratio between the hemispherical upwelling and downwelling fluxes ($F^\uparrow$ and $F^\downarrow$) at a point (Wanner et al., 1997) i.e.

$$\alpha = \frac{F^\uparrow}{F^\downarrow}$$

1.1
Albedo is a unitless quantity lying between 0 (all incoming energy absorbed) and 1 (all incoming energy reflected), and is often expressed as a percentage. Albedo is a measure of how much of the radiation incident on a surface is reflected back into the atmosphere, and consequently, how much is absorbed by the surface. If incoming solar radiation is the energy source driving all climate processes, to understand the mechanics of global climate more accurately it is vital to be able to determine the albedo of the Earth's surface as precisely as possible (Henderson-Sellers and Wilson, 1983; Mintz, 1984; Dickinson et al., 1990). Figure 1.5 is a schematic representation of the relationships driven by incoming solar radiation, which illustrates the difficulty of this task. The presence or absence of surface vegetation and cloud cover, along with atmospheric composition, are some of the critical factors affecting the rate of incoming solar radiation and emitted longwave radiation.

A wide variety of sophisticated numerical models have been developed to represent the circulation and transport processes occurring within the global climate system. Due to the importance of albedo in determining the amount of energy absorbed at the lower boundary of the atmosphere it is desirable that it should be represented as accurately as possible within any general/global circulation model (GCM) (Hall et al., 1995). Henderson-Sellers and Wilson (1983) provide a detailed review of the major GCMs in operation at the time and list the variety of different representations of albedo that are used within these models. Their conclusion is that subsequent differences between model climatologies (predicted climate outcomes based on a fixed set of starting parameters) are quite likely due to the differences in albedo. In order to remove these uncertainties, studies to obtain global albedo estimates with an accuracy of ± 5% should be initiated immediately. Henderson-Sellers and Wilson (1983) also point out that the requirement for accurate estimates of surface albedo is not a new phenomenon even in 1983, citing the GARP Joint Organizing Committee report (1975) which concludes that “there is an increasing need for reliable data concerning surface albedo”. More recently, Dickinson (1995) and Bengtsson (1995) have highlighted the continuing requirement for accurate estimates of albedo for climate models.

If there have been such demands for estimates of albedo, why have they not been met? Henderson-Sellers and Wilson (1983) list a number of the difficulties involved in generating coherent global albedo data sets:
Figure 1.5 An illustration of some of the complex interactions between incoming electromagnetic radiation, the surface and the atmosphere (after Smith, 1985).

- Spectral variation of albedo (depending on the physical structure and chemical composition of the surface).
- Angular variations of albedo leading to differences in direct and diffuse albedo. Measured albedo is assumed to lie between the two extreme cases, i) purely directional illumination conditions i.e. assuming no diffuse component of illumination (clear- or black-sky albedo), and ii) purely diffuse illumination (white-sky albedo). Consequently albedo is estimated as a function of the proportions of direct and diffuse illumination.
- Increased estimates of clear- or black-sky albedo due to a scattering atmosphere.
• Heterogeneity of the surface at various scales.

• Non-linearity of surface albedo in terms of spatial scale, necessitating generation of albedo at the correct scale for the application required (spatial interpolation and averaging are not generally appropriate).

These factors (and a number of others) combine to make albedo a very difficult parameter to determine accurately. It is still the case, however, as has been widely recognised, that satellite observations provide perhaps the best opportunity to compile global estimates of surface albedo (Henderson-Sellers and Wilson, 1983; Kimes and Sellers, 1985; Brest and Goward, 1987, Wanner et al., 1997).

1.3.3 Albedo and surface scattering

Albedo describes the ratio of upwelling to downwelling fluxes, $F^\uparrow$ and $F^\downarrow$, as expressed in equation 1.1. More exactly, albedo is defined as follows:

$$\alpha(\lambda) = \frac{\int_{\theta_i}^{\theta_i + \pi/2} \int_{\phi_i}^{\phi_i + \pi/2} L_i(\theta_i, \phi_i, \lambda) \sin \theta_i \cos \theta_i d\theta_i d\phi_i}{\int_{\theta_i}^{\theta_i + \pi/2} \int_{\phi_i}^{\phi_i + \pi/2} L_i(\theta_i, \phi_i, \lambda) \sin \theta_i \cos \theta_i d\theta_i d\phi_i} \quad 1.2$$

$L_i(\theta_i, \phi_i, \lambda)$ is the downwelling radiance in the illumination (solar) direction (solar zenith angle $\theta_i$ and azimuth angle $\phi_i$), at wavelength $\lambda$. $L_i(\theta_i, \phi_i, \lambda)$ is the upwelling radiance from the surface in the viewing direction (view zenith angle $\theta_i$ and azimuth angle $\phi_i$) at wavelength $\lambda$. $L_i$ is of course also dependent on surface reflectance. Because $L_i$ is a function of the angular distribution of downwelling irradiance, $\alpha(\lambda)$ is a function of atmospheric state and will be affected by things such as water vapour concentration and aerosol loading. Albedo should therefore not be considered an intrinsic surface property and cannot be measured directly via remote sensing. What is required for climate modelling purpose is some average, integrated hemispherical value of albedo that is independent of the atmospheric state, and is an intrinsic surface property (Wanner et al., 1997).

In order to produce such a parameter from remotely sensed data, a detailed understanding of the mechanisms determining the radiance (total incident energy) measured at the instrument is needed. This in turn requires knowledge of how the radiation incident on a surface is absorbed and scattered by that surface (ignoring for the
moment any intervening atmosphere between the surface and the sensor). More specifically, some kind of mathematical model of the surface scattering behaviour is required. If such a model can be formulated it may be possible to use the model to interpret remotely sensed observations of the surface radiance. The increasing variety and availability of remotely sensed data has driven a corresponding increase in the development of models of surface reflectance for a wide variety of applications (Goel, 1988; Asrar, 1989; Myneni et al., 1989; Hall et al., 1995; Arking et al., 1998; Knyazikhin et al., 1998a,b; Martonchik et al., 1998a,b). This thesis is concerned with one specific type of surface scattering model, developed primarily for examining predominantly vegetated land surface types.

1.3.4 Surface scattering and vegetation

One of the most important absorbing/scattering land surface types is that covered by vegetation (Dickinson, 1983; Mintz, 1984; Goel, 1988). Vegetated areas of one sort or another, from arable grazing land to tropical rainforest, cover between 50% and 70% of the Earth's land surface (Dickinson, 1983). Moreover, vegetation plays an extremely important role in global climate (Otterman, 1985; Sellers, 1989; Graetz, 1991). It provides a primary mechanism for the exchange of oxygen and carbon dioxide in the atmosphere (Schimel, 1995), regulates the transport of moisture (Shukla and Mintz, 1982) and absorbs large amounts of solar radiation for use in photosynthetic activity which may then be re-radiated into the atmosphere at a range of wavelengths. It has been shown that the time integral of photosynthetically active radiation (PAR) absorbed by vegetation canopies can be related to net primary productivity (NPP), an indicator of vegetation health, age and biomass (Steven et al., 1983; Asrar et al., 1984). NPP is primarily a measure of carbon uptake: it is the quantity of carbon fixed within vegetation (per unit area per unit time, gCm^{-2}yr^{-1}) as a net result of the transpiration minus respiration (carbon released) and photosynthesis (carbon absorbed) (Running et al., 1996). NPP has implications for global climate in terms of atmospheric CO_{2} variations (IGBP, 1998). In addition to understanding the biophysical impacts of vegetation cover on the Earth's climate, the need to monitor and develop global agriculture has provided massive economic impetus to the development of remote sensing techniques for studying vegetation. For these reasons much emphasis has been placed on attempting to understand how vegetation can be identified and monitored from remote sensing measurements. One
of the primary ways in which this has been achieved has been the development and refinement of techniques for modelling canopy reflectance ($\rho_{\text{canopy}}$) (Goel, 1989; Privette et al., 1997).

If it is possible to compute the radiant energy distribution within a vegetation canopy using a model of $\rho_{\text{canopy}}$ behaviour then a number of aims may be achieved. It may be possible to compute canopy photosynthetic rates from leaf surface projected irradiances. Hence $\rho_{\text{canopy}}$ (the exitant, measurable response of the canopy to an incident irradiance) may be calculated. This then describes the signal available for measurement from a remote sensing instrument. Models of $\rho_{\text{canopy}}$ may also be inverted against remotely measured $\rho_{\text{canopy}}$ data to enable the estimation of canopy phytometric attributes and the computation of absorbed energy (Goel and Strebel, 1983; Goel, 1989; Kustas, 1989; Sellers, 1989; Hall et al., 1995). Research into remote sensing of vegetation has long aimed to derive accurate spatial estimates of important vegetation canopy parameters such as leaf area index (LAI)$^3$, leaf angle distribution (LAD)$^4$ and fAPAR from observed $\rho_{\text{canopy}}$ data.

Figure 1.6 illustrates some of the main processes governing radiation transport within a vegetation canopy. These processes must be described accurately in order to model $\rho_{\text{canopy}}$ behaviour. Expressions relating $I^\uparrow$ and $I^\downarrow$ in figure 1.6 (upward and downward diffuse radiative fluxes, normalised by incident flux) to observed reflectance can be derived (Ross, 1975). These expressions are based on approximations and assumptions regarding canopy structural properties (3D arrangement of scattering elements within the canopy), LAI, LAD and cumulative leaf area, as well as radiometric properties (leaf reflectance, $\rho_{\text{leaf}}$, and transmittance, $\tau_{\text{leaf}}$). Canopy reflectance modelling methods are discussed in more detail in chapter 2.

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$^3$ LAI is defined as the single sided leaf area of canopy per unit ground area ($m^2$ per $m^2$).

$^4$ LAD is a function describing the distribution of leaf zenith angles within the canopy.
1.4 Surface reflectance anisotropy

"Research over the past 15 years has conclusively established that the Earth's surface is non-Lambertian, and any future analyses, excepting perhaps the most simple and crude of approximations, cannot legitimately assume Lambertian properties. Reflectance anisotropy is significant."

Conclusion drawn by Diane E. Wickland (Manager, NASA Terrestrial Ecology Programme) following NASA workshop on multiangular remote sensing for environmental applications, Jan. 29-31 1997, Univ. Maryland, (in Privette et al., 1997).
It has long been known that natural surfaces do not in general reflect incident radiation equally in all directions but instead tend to display varying degrees of anisotropy (Minnaert, 1941; Nicodemus et al., 1977; Hapke, 1981). As mentioned previously, surface reflectance is not only a function of the spectral and spatial properties of the incident radiation and target respectively, but also of the direction from which the surface is illuminated and viewed (Ross, 1981; Goel, 1988; Privette et al., 1997). The reflectance anisotropy of a surface is determined by two principal factors. Firstly, the intrinsic directionality of the spectral reflectance, transmittance and absorptance of the scattering material. Secondly, anisotropy is a function of surface roughness, or structure. The latter property is determined by the density and arrangement of objects on a surface and hence the nature of the shadowing caused by these objects as a function of illumination and observation angles (Torrance and Sparrow, 1966; Otterman and Weiss, 1982; Li and Strahler, 1986, 1992; Roujean et al., 1992). Surface structure will tend to cause incident radiation to be reflected more strongly in some directions than others. This dependence of surface reflectance on viewing and illumination geometry is described by the Bidirectional Reflectance Distribution Function (BRDF). Knowledge of the surface BRDF can therefore potentially be exploited to provide information regarding the structure of the scattering surface. Clearly, knowledge of surface reflectance is also vital in order to calculate albedo, which is intimately related to BRDF. This thesis investigates models of surface reflectance which have been developed recently in response to the need for accurate characterisation of surface reflectance at global scales.

It is clear that the anisotropic nature of the Earth's surface will have an effect on the reflectance observed from a remote sensing platform and such effects can derive from a variety of sources. Sensors possessing wide viewing swaths, such as AVHRR and MODIS, have large variations in view angle across recorded scenes (Cihlar et al., 1994; Leroy and Roujean, 1994). The same is true of sensors with along-track scanning or off-nadir pointing capabilities such as MISR, and the Along Track Scanning Radiometer instruments (ATSR and ATSR-2). Variations in the solar zenith (illumination) angle over a point on the Earth's surface will also tend to have the same effect as varying the viewing zenith angle. This occurs if a particular point is imaged at different times of day or at the same time of day throughout the year. The anisotropy of surface reflectance makes direct comparisons between such data impossible. Apparent observed changes in the nature of the surface may in fact be caused purely by variations in viewing and illumination conditions from one image to another. As the availability of time-series of
reflectance data has increased, variations caused by inconsistent viewing and illumination angles has come to be recognised as a serious problem (Leroy and Roujean, 1994; Cihlar et al., 1994).

Problems may also arise within individual scenes. Land surface process and climate modelling requirements have directed many new sensors towards global coverage at lower spatial resolution (of the order of km per pixel), and away from the high resolution observations of limited spatial coverage that have been the norm (10s of m per pixel). This is necessary in order to keep the quantities of data produced manageable. The wide swaths of such sensors such as AVHRR, MODIS and POLDER mean that there may be large variations in view angle across any single swath. MODIS for example has a swath width of approximately 2330km, with a consequent variation in view zenith of around 110° from one side to the other. So there are likely to be directional effects in observed reflectance within MODIS data simply because the viewing zenith angle varies from 0° at nadir to nearly 55° at either edge of the image. The orbital characteristics of the sensor also mean that on repeated orbits a particular point on the surface will be observed at a wide range of viewing (and illumination) angles.

Directional effects in EO data were typically ignored until relatively recently. This is exemplified by the widespread use of AVHRR maximum-value composite (MVC) products (Holben, 1985). It is now recognised that in order to make comparisons of measured surface reflectance across or between scenes, then directional effects must be accounted for (Roujean et al., 1992; Wu et al. 1994; Privette et al., 1997). In examining changes in cover type for example, comparisons must be made between data that may be separated in time by many months, and which may have been measured at significantly different viewing and illumination angles (Cihlar et al., 1994). In addition to the effects mentioned above, which are often considered as obstacles to be overcome (e.g. Roujean et al., 1992; Leroy and Roujean, 1994), the directional nature of surface reflectance can also be exploited. The directional dependence of the surface reflectance on its structural properties implies that observations of the directional component of reflectance will contain information relating to these properties (Goel and Strebel, 1983; Goel, 1988; Goel and Reynolds, 1989; Myneni et al., 1989). It may be possible to relate variations in observations at different viewing and illumination angles to the surface features causing these variations (Asrar, 1989; Pinty and Verstraete, 1991; Myneni et al., 1995).
Analogous to the manner in which spectral variations in reflectance are exploited via multi-band data, the directional component can be exploited using multi-angle data.

The fact that the directional signature of remotely sensed surfaces will contain structural information has led to the development of new missions designed specifically to explore and exploit the directional signal. This signal is not available to sensors that have no directional sampling capability, either through a wide field of view, a pointing capability or orbital characteristics. Airborne instruments such as the NASA Advanced Solid state Array Spectrometer (ASAS) (Irons et al., 1991) have been in use for some time (Barnsley et al., 1997b; Lewis et al., 1999). On a much larger scale, the MODIS and MISR instruments on-board the *Terra* platform are both specifically designed to exploit directional variations in surface reflectance (Wanner et al., 1997; Knyazikhin et al., 1998a,b; Martonchik et al., 1998a,b). MODIS data exploit the instrument's wide swath and rapid repeat coverage to provide viewing and illumination variation, whilst MISR is has nine fixed cameras, giving four look angles in the along-track direction fore and aft as well as a nadir view. An intermediate instrument is CHRIS (Compact High Resolution Imaging Spectrometer) aboard the PROBA (Project for On Board Autonomy) platform launched in autumn 2001 (Barnsley et al., 2000; www[1.11]). CHRIS is a high-resolution (25 to 50m) optical instrument which (uniquely) combines (19) selectable radiometric bands with a pointable multi-angle capability. This variety of instruments highlights the well-established (and growing) interest in multi-angle remote sensing.

### 1.5 Thesis outline

Much of the impetus for the work in this thesis derives from developments made in the design and algorithm development for a new generation of spaceborne instruments. Models of BRDF have been developed to allow both the correction of directional effects in measured reflectance data and also, more interestingly, the exploration of the directional signal. The range of approaches to modelling the reflectance of vegetation canopies has been extremely wide, with attendant variations in complexity. With MODIS already launched and entering its operational phase (and with other similar missions planned), it is becoming increasingly important to understand exactly what information can be practically and usefully extracted from the data, and how this process might be improved. This thesis presents work which is part of ongoing validation for sensor
programmes such as MODIS and CHRIS, as well as contributing to the understanding of existing algorithms and the development of new ones.

Chapter 2 contains a theoretical discussion of BRDF as well as a review of important concepts and developments in surface reflectance modelling. In particular, simple semi-empirical kernel-driven models of BRDF developed specifically for use with the MODIS sensor are introduced. These models are an important development for near real-time production of the type of global, moderate resolution products required for the study of global climate processes. The kernel-driven models are just starting to be used operationally to produce estimates of albedo and burn scar area from surface reflectance. This thesis explores how these relatively simple models can apparently describe the complex scattering behaviour of vegetation canopies at a range of scales. In addition, the nature of biophysical information contained in the model parameters is explored and potential improvements and extensions of the modelling concept are proposed.

Chapter 3 is a description of fieldwork carried out to obtain a variety of plant canopy data. Detailed 3D models of canopy structural and radiometric properties are generated from structural measurements and subsequently used to simulate values of canopy reflectance, \( \rho_{\text{canopy}} \). The simulations of \( \rho_{\text{canopy}} \) are the basis for exploration and understanding of the assumptions underlying certain canopy reflectance modelling techniques. Contemporaneous measurements of a variety of canopy parameters made during the field campaign are used to validate simulated values of \( \rho_{\text{canopy}} \).

Chapter 4 describes a set of experiments intended to establish the validity of the semi-empirical kernel-driven approach to modelling BRDF. Values of \( \rho_{\text{canopy}} \) are simulated under the assumptions made in the formulation of the linear kernel-driven models and the results are used to explore these assumptions. The assertion that \( \rho_{\text{canopy}} \) can be separated into its constituent scattering components is examined. Results show that the separate components of simulated \( \rho_{\text{canopy}} \) do in general describe what they are purported to in the model formulation.

Chapter 5 explores the relationship between the linear kernel-driven model parameters and the corresponding scattering components derived from the 3D canopy simulations. The assumptions underlying the linear kernel-driven models are tested and situations where these assumptions may break down are highlighted. This is the first time
that these assumptions have been tested explicitly, rather than being inferred from the ability of the kernel-driven models to fit observed reflectance data.

**Chapter 6** contains an analysis of the information content of the model parameters. Results show that model parameters may contain biophysical information that can be exploited but it may be coupled with other information. This indicates that the model parameters should be interpreted with great care, particularly in the absence of other ancillary information. Model parameters may have an indirect use for analysis such as land cover classification or change detection.

**Chapter 7** presents a new extension of the linear kernel-driven modelling approach into the spectral domain. Such an approach appears to offer significant improvements over current kernel-driven models, which are limited to the angular domain. This is particularly true for the derivation of products such as broadband (across visible and NIR wavelengths) albedo from narrowband spectral samples. So-called 'spectral kernels' are derived and tested against simulated (and measured) reflectance data.

**Chapter 8** contains conclusions drawn from the experimental results presented in the thesis and discusses directions for further research. In particular, further developments of the spectral kernels are proposed and plans are outlined for the application of a full spectral directional kernel-driven model of the type developed in chapter 7 to airborne and spaceborne data.
2 Review of BRDF and canopy reflectance modelling

Liang et al. (2000a) review the current state of multi-angle remote sensing following the International Forum on BRDF (IFB), San Francisco, December 1998. They conclude that multi-angle remote sensing, at the threshold of the EOS era, is now yielding data which are set to provide unique insight into surface biogeophysical processes.

Radiation reflected from the Earth’s surface is characterised by a small number of key signatures (or domains of information) (Gerstl, 1990; Liang and Strahler, 1994):

1. **Spectral** ($\lambda$): reflectance, transmittance and absorptance response of canopy elements to radiation of different wavelengths (Jacquemoud and Baret, 1990; Curran et al., 1992).

2. **Spatial** ($x, y$): e.g. spatial structure at the macroscopic level (objects are much larger than the wavelength of incident radiation), arrangement of scattering objects on a surface, appearance of target at different scales, adjacency, mixed pixels (Woodcock et al., 1988).

3. **Temporal** ($t$): e.g. seasonal change of vegetation growth profiles; inter-annual variability of vegetation quantity (Myneni et al., 1997).

4. **Angular** $\Omega(\theta, \phi), \Omega'(\theta, \phi)$: reflectance anisotropy caused by surface structure e.g. hotspot – the peak of reflectance in retro-reflection direction (viewing and illumination vectors, $\Omega$ and $\Omega'$, are near coincident) (Ross, 1981; Kuusk, 1985).

5. **Polarization** $p(\phi)$: e.g. polarization information contained in surface reflectance signal (Vanderbilt et al., 1985; Deschamps et al., 1994).

6. **Time-resolved** ($\partial T$): time-resolved returns from active instruments, such as optical (laser) LiDAR (Light Detection And Ranging), and phase information from microwave RADAR (Radio Detection and Ranging) instruments ($\lambda$ of the order of cm).
The intrinsic surface reflectance is a function of all of these signatures, but differs from the signal measured at the sensor due to the effects of atmosphere, sensor response etc. Exploration of the first three signatures above has formed the basis of conventional remote sensing (Goel, 1988; Gerstl, 1990). The fifth component has only been deliberately exploited recently with the advent of the (now-defunct) POLDER, and forthcoming POLDER II instruments (Deschamps et al., 1994; Leroy et al., 1996). The sixth component has also been exploited only relatively recently: LiDAR is currently being explored as a new method of obtaining information on surface properties, particularly vegetation canopy structure (www[2.1]). Phase information from RADAR instruments can be used to determine information regarding the structure and scattering behaviour of the surface (Sun and Ranson, 1995; Saich et al., 2001).

The directional signal (4) has historically been one of the least exploited of these signatures (Goel, 1992; Liang and Strahler, 1994; Myneni et al., 1995; Privette et al., 1997) and was until relatively recently mostly ignored. Barnsley et al. (1997a) have shown that multiple view angle (MVA) data contain information entirely separate from the spectral component of measured reflectance. This indicates that the directional signal can be used to distinguish between cover types purely on the basis of surface structural detail, even where spectral responses are identical (Asner, 2000). This thesis is primarily concerned with the information content of the directional signature, but also examines the possibility of extending and including spectral information into simple directional modelling methods.

Considering the reflectance signal from a vegetation canopy, Goel (1992) extends the description by Gerstl (1990) given above to propose the following functional description of the relationship, R, between the measured spectral directional reflectance \( \rho \) of a vegetation canopy, and the parameters controlling that signature:

\[
\rho = R(\lambda, t, (x, y), (\Omega, \Omega'), P, \theta T; C)
\]

In addition to the five signatures described above, R is also dependent on a set of canopy parameters, C, representing the characteristics of the canopy and its underlying surface (soil, snow etc.) contributing to the form of \( \rho \). In order to derive information regarding vegetation from measurement of reflectance, models of vegetation canopy reflectance (CR) are constructed (Goel, 1988). A model of CR is an attempt to i) formulate an accurate forward relationship to predict \( \rho \) for given R and ii) determine C from measured
\( \rho \) (at given values of \( \lambda, t, (x,y), (\Omega, \Omega'), \partial T, P \)) i.e. to invert (or understand) the canopy parameters from the relationship in equation 2.1.

The development of EO as a powerful tool for monitoring and mapping the global environment has been introduced in chapter 1. This chapter discusses the implications of the anisotropic nature of surface reflectance under variable viewing and illumination conditions. The potential for exploitation of the directional nature of surface reflectance through the application of canopy reflectance models is explored. Mathematical techniques for the inversion of such models against measured reflectance data are introduced. Following this a review of some of the many available canopy reflectance modelling (CR) techniques is undertaken. The conclusion of this is the introduction of a particular class of canopy reflectance models, developed for their simplicity and effectiveness, which are to be used to derive products from forthcoming sensors such as MODIS and MISR. Experimentation in subsequent chapters explores the potential for these models to extract information regarding vegetation canopies from reflectance data in practice.

2.1 Factors affecting surface reflectance anisotropy

The size, shape and distribution of objects on a surface have a direct impact on the nature of the radiation scattered from the surface (Hapke, 1981, 1993). The measured reflectance signal is therefore a function of surface structure. Vegetation is one of the most important absorbing/scattering land surfaces that can impact a remote sensing signal (Asrar, 1989; Myneni and Ross, 1990; Sellers, 1992; Asner, 1998). Examples of important biophysical parameters such as LAI, fAPAR and albedo, which are used by ecologists, climatologists and remote sensing scientists to describe the quantity and influence of vegetation, were introduced in the previous section.

Vegetation plays an extremely important role in the global climate (Dickinson, 1983, 1995; Otterman, 1985), providing a primary mechanism for the exchange of \( \text{O}_2 \) and \( \text{CO}_2 \) in the atmosphere (Schulz et al., 2001; Zhan and Kustas, 2001), as well as energy fluxes through photosynthetic activity (Ross, 1981; Verstraete, 1987), moisture fluxes (Shukla and Mintz, 1982) and transfers of momentum (Sellers, 1995). Indeed, Asner (2000) notes "MVA remote sensing measurements are uniquely sensitive
to variation in key structural characteristics of vegetation, soils and atmospheric constituents". For these reasons, much emphasis has been placed on attempting to understand how vegetation can be detected and monitored from remote sensing measurements. One of the primary ways in which this has been achieved has been the development and refinement of CR modelling techniques (Allen et al., 1970; Ross, 1981; Goel, 1988; Asrar, 1989; Privette et al., 1997; Strahler, 1996).

It is well-known that natural surfaces are generally not Lambertian reflectors (i.e. reflecting incident radiation equally in all directions), but will tend to display varying degrees of anisotropy (Minnaert, 1941; Nicodemus et al., 1977; Hapke, 1981). Surface reflectance is therefore not only a function of the spectral, spatial and polarising properties of the target, but also of the direction from which the surface is illuminated and viewed (Ross, 1981; Goel, 1988). Measured reflectance (as opposed to the intrinsic surface reflectance) will also be dependent on the spectral and directional nature of the irradiance. The directional nature of surface reflectance is illustrated in figure 2.1.

![Figure 2.1](image.png)

**Figure 2.1** Four examples of surface reflectance: (a) Lambertian reflectance (b) non-Lambertian (directional) reflectance (c) specular (mirror-like) reflectance (d) retro-reflection peak (hotspot).
The degree to which incident radiation from a surface is reflected anisotropically is determined by factors such as the density and arrangement of objects on the surface, and hence the nature of the shadowing caused by these objects as a function of viewing angle, illumination zenith and azimuth angles, \( \theta_v \) and \( \phi_v \), respectively (Otterman and Weiss, 1982; Li and Strahler, 1986, 1992; Roujean et al., 1992), as well as the intrinsic directionality of the reflectance, transmittance and absorptance properties of the scattering materials (Asrar, 1989). Reflectance anisotropy can also be a function of the aggregated scattering properties of objects. The existence of surface structure tends to cause the surface to depart from Lambertian and, as a result, incident radiation is reflected more strongly in some directions than others. This directionality of surface reflectance can potentially be exploited to provide information regarding the surface structure. This is illustrated by the specular and hotspot peaks shown in figure 2.1c and d. The hotspot peak arises because a minimum of shadowed surface is viewed when the viewing and illumination vectors are collinear (Hapke, 1984). This is a characteristic feature of vegetation canopy reflectance and is related to the size and distribution of scattering objects within the canopy (Kuusk, 1985; Pinty and Verstraete, 1992). The next step is to introduce a formal description of surface reflectance anisotropy.

### 2.1.1 Bidirectional reflectance distribution function (BRDF)

Figure 2.1 illustrates the tendency of natural surfaces to reflect incident radiation anisotropically. This behaviour is formally described by the (spectral) bidirectional reflectance distribution function (BRDF) (Nicodemus, 1970; Nicodemus et al., 1997; Hapke, 1981). The BRDF of a small surface area \( \delta A \) (at a particular wavelength of non-polarised) illuminating radiance) is defined as the ratio of the incremental radiance leaving the surface through an infinitesimal solid angle in the direction defined by the viewing vector, \( \Omega(\theta_v, \phi_v) \) (where \( \theta_v, \phi_v \) are the viewing zenith and azimuth angles) to the incremental irradiance from direction defined by the illumination vector, \( \Omega'(\theta_i, \phi_i) \) (where \( \theta_i, \phi_i \) are the illumination zenith and azimuth angles). This is expressed in equation 2.2 (ignoring any dependence of BRDF on wavelength, \( \lambda \))

\[
BRDF(\Omega, \Omega') = \frac{dL_e(\Omega, \Omega')}{dE_i(\Omega')} \quad [sr^{-1}]
\]

Where \( dL_e \) is the incremental radiance reflected from the surface into the differential solid angle in the viewing direction \( \Omega \) (Wm\(^{-2}\)sr\(^{-1}\)) (Nicodemus et al., 1977; Martonchik et al.,
Figure 2.2 Configuration of viewing and illumination vectors in the viewing hemisphere, with respect to an element of surface area, $\delta A$.

Equation 2.2 only deals with two of the domains of information described in the expression for measured reflectance given in equation 2.1, but for exploring spectral directional reflectance these are the important ones. BRDF as defined in equation 2.2 is a fundamental property of the surface, describing the intrinsic surface reflectance. However, it is defined only for infinitesimal viewing and illumination solid angles and an infinitesimal wavelength interval. Consequently it cannot be directly measured. In EO applications, illumination is typically over a hemisphere with both direct and diffuse sources (solar illumination, and sky radiance respectively). Viewing is typically over some finite sensor instantaneous field-of-view (IFOV), defined by the sensor optics and geometry, with a spectral response over some finite wavelength interval rather than at some discrete value of $\lambda$.

In practice, it is assumed that the BRDF can be retrieved with some level of uncertainty, from radiance measurements over the IFOV using a collimated beam light source (e.g. laser or direct sunlight). In this case, BRDF is the limit case of biconical reflectance measurement. To overcome the problem that the BRDF is a non-measurable property, we define a bidirectional reflectance factor (BRF) $\rho(\lambda, \Omega, \Omega')$, which is the ratio of radiance leaving the surface in a finite solid angle in the viewing direction $\Omega$ to the
radiance from a perfect Lambertian reflector under the same illumination conditions as the target, into the same finite solid angle i.e.

$$\rho(\Omega, \Omega', L_{\text{sky,sun}}(\Omega, \Omega')) = \frac{L_e(\Omega, \Omega', L_{\text{sky,sun}}(\Omega, \Omega'))}{L_{\text{Lambertian}}(\Omega, \Omega', L_{\text{sky,sun}}(\Omega, \Omega'))}$$  \hspace{1cm} 2.3$$

where $L_e$ is the radiance exitant from the surface (Wm$^{-2}$sr$^{-1}$); $L_{\text{Lambertian}}$ is the radiance from a perfect Lambertian reflector (Wm$^{-2}$sr$^{-1}$); $L_{\text{sky,sun}}$ are the sky and sun radiance distributions (Wm$^{-2}$sr$^{-1}$). It can be seen that the BRF is dimensionless.

As a result of the incident irradiance and exitant radiance being defined over infinitesimal solid angles $\delta\Omega$ and $\delta\Omega'$, BRF can be calculated as an integrated property i.e. the numerator in equation 2.2 becomes:

$$L_e(\Omega, \Omega', E_i(\Omega, \Omega'), L_{\text{sky,sun}}(\Omega, \Omega')) = \int_0^{2\pi/2} \int_0^\pi \rho_s(\Omega, \Omega') \sin \theta \, d\theta \, d\phi$$  \hspace{1cm} 2.4$$

where $\rho_s$ is the surface reflectance function (BRDF); $d\Omega = \cos \theta \sin \theta \, d\theta \, d\phi$ (and similarly for $d\Omega'$. It can be seen from equation 2.3 that in order to derive the exitant radiance, the viewing and illumination vectors are integrated over the respective viewing and illumination hemispheres. In the same way, the radiance from the Lambertian surface is defined as

The integral is purely over the illumination direction as the observed reflectance, by definition, is the same regardless of the viewing direction. In practice, the BRF is often defined as the radiation exiting the scene in a given direction (an infinitesimal angle), rather than as an integrated property. If a point illumination source is considered i.e. no sky irradiance, then, for this case

$$BRF(\Omega, \Omega') = \pi BRDF(\Omega, \Omega')$$  \hspace{1cm} 2.6$$

The expression in equation 2.6 utilises the fact that the BRDF of perfect Lambertian reflector is $1/\pi$. This is due to the fact that a perfectly diffuse surface reflects the same radiance, $E_i(\theta_i)/\pi$ in all directions. As a result, the BRF of any surface is equal to its BRDF multiplied by $\pi$.

Practically, measured surface reflectance is a function of the direct and diffuse component of incident irradiance (rather than being an intrinsic surface property).
Consequently, integrals of the BRDF over the viewing and illumination hemispheres are defined. The directional hemispherical reflectance (or DHR), $\rho(\Omega,\Omega')$, is the integral of BRF over the viewing (or illumination) hemisphere. It is the hemispherical reflectance assuming a directional (collimated beam) illumination source (or alternatively, the directional reflectance for a diffuse illumination). This can be expressed as:

$$\bar{\rho}(\Omega';2\pi) = \frac{1}{\pi} \int_{\epsilon}^\pi BRDF(\Omega,\Omega')d\Omega$$

This expression defines the so-called black-sky albedo (Wanner et al., 1995) i.e. it defines the hemispherical reflectance under conditions of purely directional illumination (no sky radiance). $\bar{\rho}(\Omega')$ can be integrated over all illumination directions to yield $\bar{\rho}$ the bihemispherical (or hemispherical-to-hemispherical) reflectance (or BHR). This is the reflectance of a surface over all viewing angles due to a diffuse illumination source i.e.

$$\bar{\rho}(2\pi;2\pi) = \bar{\rho}(\Omega')d\Omega' = \frac{1}{\pi} \int_{\epsilon}^{2\pi} \int_{\epsilon}^{2\pi} BRDF(\Omega,\Omega')d\Omega d\Omega'$$

which is the so-called white-sky albedo i.e. the hemispherical reflectance under perfectly diffuse illumination conditions.

It is important in the context of remote sensing applications to note that BRDF cannot be directly measured because:

i) (from equations 2.2 and 2.3) BRDF is defined as the ratio of two partial derivatives and BRF is defined as reflectance relative to that of a perfect Lambertian reflector.

ii) No sensor has a perfectly discrete spectral response, and so measurement of BRDF is inevitably a convolution of the signal with the sensor spectral response function over a range of wavelengths. Additionally, the projected instantaneous IFOV of the sensor must be accounted for i.e. measurement is not over an infinitesimal angle.

iii) In practice, observations are made through some depth of atmosphere so that the measured signal is also a function of atmospheric absorption and scattering (reflectance and transmittance). To retrieve measures of surface reflectance through the atmosphere, the scattering behaviour of the
atmosphere (and in particular the scattering phase function) must be
careracterised accurately.

Using the relationships in equations 2.2-2.8 it is now possible to relate BRDF to
albedo. The BRDF explicitly describes the directional nature of exitant radiation from a
surface. As a result, albedo, the total irradiant energy (both direct and diffuse) reflected in
all directions from the surface, is an integrated measure of the directional reflectance over
the viewing/illumination hemisphere. Albedo is thus a function of the quantities of diffuse
and direct illumination arriving at the surface. In the discussion above, dependence of
BRDF on $\lambda$ has not been considered. In practice, BRDF is also a function of $\lambda$. Typically
reflectance data are either reported as a function of $\lambda$, or the finite wavelength interval
over which the parameters have been integrated during observation is specified. In such
instances, parameters such as BRF, DHR and BHR are should be prefaces by "spectral"
or "narrowband".

Further approximations are required in practice in order to relate estimates of
albedo made at narrow wavelength bands (narrowband) to total albedo over the visible
and NIR regions of the spectrum (broadband). This has been discussed by a number of
researchers, in a variety of ways (Stephens et al., 1981; Stum et al., 1985; Kimes and
Sellers, 1985; Cess and Potter, 1986; Brest and Goward, 1987; Koepke and Kriebel,
1987; Dickinson et al., 1990; Liang et al., 1999). Spectral albedo $\alpha(\lambda)$ can be
approximated as a combination of the two components of black-sky and white-sky albedo
(Wanner et al., 1997; Strugnell and Lucht, 1999), weighted by $D$, the proportion of
diffuse illumination from the atmosphere i.e.

$$
\alpha(\lambda) = (1 - D(\lambda, \Omega', \tau))\bar{\rho}(\lambda, \Omega') + D(\lambda, \Omega', \tau)\bar{\rho}(\lambda)
$$

2.9

where $D(\lambda, \Omega', \tau)$ is function of the illumination conditions and the atmospheric state,
characterised by the atmospheric optical depth, $\tau$. Equation 2.9 is a reasonable
approximation to spectral albedo except at high solar zenith angles (Lewis and Barnsley,
1994). The total surface albedo, $\alpha$ i.e. the ratio of the total incident shortwave radiation to
the reflected radiation can then be approximated as an integral over all shortwave (SW)
radiation (ignoring anisotropy of incident diffuse radiation) i.e.

$$
\alpha = \int_{SW} p(\lambda) \alpha(\lambda) d\lambda
$$

2.10
where \( p(\lambda) \) is the proportion of illumination in the solar spectrum, dependent on the atmospheric state. \( 1 - \alpha \) is then the proportion of incident shortwave radiation absorbed at the surface (stored as heat energy and chemical energy through photosynthesis). Application of the method to EO data requires the integral over all SW to be approximated with a weighted sum of the available wavebands (Lewis et al., 1999), or through the use of other modelling techniques (Liang, 2000; Lucht and Roujean, 2000). This limitation will be discussed in later chapters.

The properties defined above can be measured in practice. To characterise up- and downwelling radiation fluxes from the surface a description of the surface scattering behaviour is required. Indeed, surface properties cannot be related to measured radiance without such a model. Many models describing the scattering of radiation by vegetation have been developed; some to correct angular dependencies (Roujean et al., 1992; Cihlar et al., 1994 Liang et al., 2000b), some to relate canopy scattering behaviour to remote measurements of reflectance (e.g. Goel and Strebel, 1983; Goel 1988, 1992; Nilson and Kuusk, 1989; Pinty and Verstraete, 1991). An overview of these methods is given in section 2.5.

2.1.2 Removal of reflectance anisotropy effects from observed reflectance

Reflectance anisotropy arises in a variety of ways. Sensors possessing wide viewing swaths such as AVHRR, with a swath width of 2500km, have variations in view angle across scenes (70° in the case of AVHRR) (Leroy and Roujean, 1994; Cihlar et al., 1994; Li et al., 1996). In addition, a point on the surface may be located in different parts of the viewing swath on subsequent orbits, and will therefore be viewed from different angles. This is also true for sensors with along-track scanning or off-nadir pointing capabilities such as ATSR-2 (North et al., 1999) POLDER (Deschamps et al., 1994), and the forthcoming CHRIS instrument (Barnsley et al., 2000). This is schematically illustrated in figure 2.3. Surface reflectance is also dependent on the solar zenith angle. This is manifested if a point on the Earth’s surface is viewed at different times of day, for example from a geostationary viewing platform such as METEOSAT, or is viewed on different days from a polar orbiting platform such as AVHRR. Sun-synchronous observations will also tend to be affected by the annual cycles of variation in solar zenith angle.
angle. Liang et al. (2000b) review recent developments in the angular correction of BRDF data, in particular for modelling surface energy fluxes, and in particular, albedo.

With the increase in availability of large satellite data sets, the reflectance variations caused by inconsistent viewing and illumination angles has come to be recognised as a serious problem (Kimes et al., 1980; Royer et al., 1985; Leroy and Roujean, 1994; Cihlar et al., 1994). Assuming that the Earth’s surface is Lambertian and ignoring directional effects will introduce significant errors in estimates of surface reflectance from EO data. In order that observations separated in time by many months and measured at significantly different viewing and illumination angles may be compared, directional effects must be accounted for (Lee and Kaufman, 1986; Roujean et al., 1992; Wu et al. 1994; Privette et al., 1997a). This may be achieved by normalising reflectance measurements to a standard viewing and illumination equivalent reflectance which permits intercomparison of data obtained at varying sun and view zenith angles (Gutman, 1994). It is now recognised that viewing and illumination angle effects should be considered significant: reflectance observations made at different viewing and illumination angles are not directly comparable, even if all other things are considered equal (Privette et al., 1997; Roy et al., 2001).
2.1.3 Reflectance anisotropy as a source of information

In contrast to the undesirable effects described above, the directional nature of surface reflectance can also be exploited as a source of information. The directional dependence of surface reflectance on structural properties implies that observations of the directional signal will contain information relating to these properties (Goel and Strebel, 1983; Goel, 1988; Myneni et al., 1989; Pinty and Verstraete, 1991). If it is possible to relate radiant energy from a vegetation canopy to observed reflectance using a model of some kind, then it may also be possible to use such a model to relate variations in observed reflectance to surface properties causing these variations (Asrar, 1989; Pinty and Verstraete, 1991; Myneni et al., 1995; Asner, 2000). Such a relationship can be used to normalise directional effects in directional data sets, as discussed above (Roujean et al., 1992; Cihlar et al., 1994; Liang et al., 2000b). More usefully for the study of vegetation characteristics however, such a model may be inverted against measured reflectance data to provide estimates of model parameters (Goel and Strebel, 1983; Pinty and Verstraete, 1990, 1992; Hall et al., 1995; Liang et al., 2000a). If the model parameters describe surface properties, such as the size and distribution of scattering objects say, then estimates of these surface properties may be obtained. This thesis is concerned with recent developments in modelling surface scattering from vegetation, which are now being used to produce land-cover products from recent and forthcoming instruments. Before describing methods of CR modelling however, attention must be paid to the effect of the atmosphere on remotely sensed measurements.

2.2 Atmospheric effects on measured surface reflectance

Reflected solar radiation measured at a remote sensing platform must travel through the Earth's atmosphere both on the way down from the direction of the sun, and on the way back up to the measuring platform. The intervening atmosphere contains various gases and aerosols, which absorb and/or scatter upwelling and downwelling radiation. The most abundant atmospheric gas in terms of absorption of incoming radiation is water vapour (contributing approximately 75% of the global greenhouse effect), which absorbs radiation strongly in the NIR and mid-IR regions (Salby, 1995). In addition, the atmosphere contains aerosol particles such as sulphates, mineral dust, soot and sea salt, originating from sources such as volcanic eruption, industrial and urban
emissions or oceanic evaporation. These aerosols can have significant scattering effects (Rayleigh and Mie, depending on particle diameter) and cause the signal received at the sensor to be attenuated (Kaufman, 1989; Vermote et al., 1997a,b). This can be particularly important when investigating surface properties such as albedo (Lyapustin, 1999). Atmospheric gases and aerosols can also be highly temporally and spatially variable and are therefore difficult to characterise accurately (Martonchik et al., 1998a). This behaviour is generally characterised by the aerosol optical depth, \( \tau \) (Zibordi and Voss, 1989).

**Figure 2.4** Four sources of atmospheric perturbation to the measured surface reflectance signal.

Figure 2.4 illustrates four sources of atmospheric scattering that cause perturbation of the surface reflectance signature. \( R_1 \) is incoming radiation reflected towards the sensor by a single scattering interaction in the atmosphere. \( R_2 \) is incoming radiation scattered first from the surface outside the target area then by the atmosphere into the path of the sensor. \( R_3 \) is incoming radiation scattered by the atmosphere onto the target and then to the sensor. \( R_4 \) is incoming radiation scattered from the surface outside the target, then by the atmosphere above the target back on to the target, then to the
sensor. Note in R4 that a component of the signal reaching the sensor will contain radiation reflected from the area surrounding the target in addition to the desired signal (Kaufman, 1989). There are obviously more complex interactions if higher orders of scattering between the surface and atmosphere are considered. These will tend to be successively smaller in magnitude than the single scattered interactions due to attenuation by absorption, scattering and transmission at each successive interaction, and will also tend to be isotropic (Vermote et al., 1997a,b). If information regarding the scattering behaviour of the target is sought, this extraneous atmospheric signal which acts to ‘blur out’ the surface reflectance signal, must be accounted for. It is clear that the atmosphere adds significantly to the path radiance at red wavelengths (and even more so at shorter wavelengths), whilst attenuating the surface reflectance at IR wavelengths (Kaufman, 1989; Myneni et al, 1993).

In order to isolate the desired surface signal, the contribution of the intervening atmosphere must either be removed (as far as possible) or modelled as part of the signal through the application of a coupled model of surface-atmosphere scattering. Removing the atmospheric perturbation of measured surface reflectance is typically performed using a model of the scattering behaviour of the atmosphere (coupled with some assumption of surface reflectance behaviour). The Second Simulation of the Satellite Signal in the Solar Spectrum (6S) code of Vermote et al. (1996) for example, uses available ozone and water vapour concentrations, aerosol optical depth at 550nm, knowledge of sensor response and atmospheric pressure and a model of surface reflectance properties to generate parameters which allow surface reflectance to be calculated from at-sensor top-of-atmosphere (TOA) radiance values. There are a number of other models for the atmospheric correction of measured radiance data such as those of Rahman and Dedieu (1994) and Berk et al. (1992). Kaufmann (1989) gives a comprehensive review of methods that have been developed in order to account for the atmospheric component of remote measurements of the Earth’s surface.

The second approach to accounting for atmospheric effects is based on the observation that the measured directional reflectance signal is a function of both the surface and the atmosphere and the coupling between them (Myneni and Asrar, 1993). A number of combined surface-atmosphere models have been developed in order to characterise this coupling. Liang and Strahler (1993) described the coupled atmosphere-canopy system as two plane-parallel layers with a non-Lambertian soil boundary. The
the total radiation field in this case is calculated by treating the unscattered, single scattered and multiple scattered radiation separately. A similar approach is taken by Rahman et al. (1993a, b) in their coupled surface-atmosphere reflectance (CSAR) model. Their results show that the BRDF signal undergoes smoothing as a result of atmospheric effects, thus emphasising the importance of considering the coupling between surface and atmosphere. Lewis et al. (1999) demonstrate that both the magnitude and (more importantly) the shape of the surface BRDF can be completely mis-estimated if atmospheric correction is not performed accurately. In particular, the correct choice of scattering phase function is shown as crucial in maintaining the surface reflectance shape. Lyapustin (1999), and Lyapustin and Privette (1999), have shown the importance of the accurate characterisation of atmospheric absorption and scattering in the derivation of albedo from multi-angular measurements. Interestingly, Lyapustin (1999) has recently shown that there appears to be a small, well-defined range of solar zenith angles between approximately 52° and 57° where surface albedo is almost insensitive to atmospheric opacity.

Atmospheric correction of remotely sensed data has generally been performed on a 'per scene' basis, ignoring spatial variability within scenes and assuming a uniform Lambertian surface (Tanré et al., 1986; Fraser et al., 1992). Typically, the total radiation flux from the top of the atmosphere (TOA) to the surface is described as the sum of direct and diffuse components – the latter caused by absorption and transmission of atmospheric gases such as water vapour and scattering by atmospheric aerosols. The assumption of Lambertian surface reflectance is made in order to simplify the calculation of radiation scattered multiply between the surface and atmosphere. Lee and Kaufmann (1986) demonstrate that this assumption can cause significant errors in the retrieval of surface reflectance, particularly in the backscattering direction and for large illumination angles (60° and above) due to coupling between surface reflectance and the atmosphere. Hu et al. (1999) state that such errors can be from 2-7% up to 15% in the worst case. As a result, when investigating directional reflectance variations, a more spatially accurate approach requiring per-sample (per pixel, depending on pixel resolution) corrections is required (Vermote et al., 1997a). The additional computational effort required to achieve this is a major limitation on the rapid processing of large data sets. Recent instruments designed to measure surface reflectance variations (e.g. MODIS and POLDER) have been developed to use a variety of data regarding the state of the atmosphere and the surface surrounding the target in order to produce improved atmospheric corrections.
Atmospheric correction developed for the MODIS surface reflectance product for example, assumes that the signal at the sensor is a distance-weighted sum of the contributions from the pixels surrounding the target (Vermote et al., 1997a,b). Measurements of ozone, water vapour and pressure are also used in calculating atmospheric attenuation of the measured signal. Simultaneous multi-angle measurements of the surface during a single overpass from sensors such as MISR (Martonchik et al., 1998) and CHRIS (Barnsley et al., 2000) provide another possibility. The (now defunct) POLDER instrument was designed to measure the polarisation of incoming radiation in order to characterise the atmospheric aerosol scattering phase function. This information can be used to further improve the atmospheric correction process by identifying the various types and concentrations of scattering particles (Leroy et al., 1996).

It has been shown that the atmosphere between target and sensor contributes significantly to the difficulty of measuring surface BRDF remotely. As such, it is desirable to account for the scattering behavior of the atmosphere in some way. However, it should also be noted that the scattering caused by atmospheric aerosols is a valuable source of information in its own right. Clearly, if radiation reflected from surface to sensor is attenuated due to atmospheric scattering, the same must also be true for incoming solar radiation. In fact, atmospheric aerosols play a major role in the Earth’s radiation budget (Charlson et al., 1992; Kiehl and Briegleb, 1993). Tropospheric aerosols (and associated indirect effects) are thought to contribute of the order of 1Wm$^{-2}$ to atmospheric radiative forcing (IPCC report, 1995). The effects are not well understood, however, owing to the inherent spatial and temporal variability of atmospheric aerosols, combined with uncertainty regarding tropospheric composition of aerosols and their single scattering albedo and phase function. This is a severe barrier to understanding the impact of atmospheric aerosols on global climate.

As a consequence of the poor quality of available knowledge of atmospheric aerosol distribution and scattering behaviour, instruments such as MISR are now generating information regarding atmospheric aerosol concentration and type (Martonchik et al., 1998a). Rather than attempt to compensate for the scattering behaviour of the atmosphere, the nine cameras of the MISR instrument (four spectral bands) characterise atmospheric scattering at the various path lengths experienced by each camera. Pre-determined aerosol mixture models have been used in conjunction with radiative transfer models of scattering behaviour to pre-calculate TOA radiance values.
These are compared with measured radiance values in order to invert the actual aerosol scattering properties on a global scale. It is hoped that the creation of a detailed aerosol climatology will enable a far more accurate characterisation of the impact of aerosol forcing on global climate than has so far been possible. Further, it is notable that the use of multi-angle imaging (e.g. MISR, ATSR etc.) can be used to overcome the difficulty of separating the components of surface and atmospheric reflectance inherent in the measured signal.

2.3 Canopy reflectance: The forward and inverse problems

Monitoring vegetation using remotely measured data is a problem of the sort occurring in the observation of almost any complex physical system (Twomey, 1977; Gershenfeld, 1999). The solution in general is to construct a model of the system. If the model describes the interactions of the system sufficiently well (i.e. to some desired level of accuracy), then the model can be used to describe the outcome of the system based on chosen inputs. This is described as running the model in ‘forward’ mode or ‘forward modelling’ (Goel, 1992). If the model predictions are in agreement with the observed behaviour of the system, we can have some degree of faith in the ability of the model to predict the behaviour of the system under arbitrary input conditions. An important caveat is that no matter how good the agreement between the modelled and measured state of the system, the model can never truly be ‘validated’. It is always prone to the twin problems that natural systems are never closed and that model results are always non-unique (Oreskes et al., 1994). The primary cause of non-closedness in a natural system is ‘noise’: unwanted perturbations of the desired signal by factors outside immediate consideration. For example, the intervention of the atmosphere between the surface and a remote sensing instrument causes perturbation of the observed reflectance, as does the imperfect spectral response of the sensor. As a result, a single point on the Earth’s surface may appear to have quite different reflectance if observed on different days, at different times of day or from different sensors. These effects can be modelled (Lucht and Lewis, 1999) but other factors such as the difficulty of accurately characterising generalised parameters and the sensitivity of the model inversion process to sampling (spectral and directional) conspire to make model validation difficult. This is an ever-present problem that must always be addressed carefully in modelling natural systems (Justice et al., 2000).
Figure 2.5 Schematic representation of forward and inverse modes of $\rho_{\text{canopy}}$ model operation (solid lines represent the model in forward mode; dashed lines and blue boxes represent path taken during model inversion).

Having a forward model that adequately describes the state of a system is useful in that it may allow predictions on the future state of the system to be made. However, what is often of most interest is the set of parameters governing the system. How can information regarding these parameters be derived from the model? The solution is to ‘invert’ the model (or run the model in ‘inverse’ mode). This implies making observations of the system and then manipulating the model parameters so that the outputs of the model match the observations as closely as possible. It can then be postulated that the resulting parameter values are the values that cause the system to be in the measured state. This explanation relies on the fact that for any particular model state there exists a unique set of driving parameters (which in practice is never the case due to noise). However, model inversion against reflectance data provides a very powerful method of deriving information about canopy parameters from remote measurements. The generic forward and inverse process is illustrated schematically in figure 2.5. The solid arrows in figure 2.5 represent the modelling process for linear systems, which can be inverted analytically. The dashed lines represent the iterative inversion process that is typically required to invert a non-linear model of $\rho_{\text{canopy}}$. The experimental work presented in this thesis aims to investigate the possibilities for vegetation canopy parameter retrieval from measured reflectance data, primarily using linear models developed for the MODIS sensor (Wanner et al., 1995, 1997). To fully understand the way in which such models
can be applied, and the type of information it may be possible to retrieve, a good understanding of the various methods of model inversion, both linear and non-linear, is required.

2.4 Mathematical approaches to model inversion

There are many ways of inverting mathematical models. In simple linear systems an analytical solution may be found to the problem of inversion (ignoring for the moment any uncertainty due to noise in the observations) as long as the system is determinate. This implies the system is neither underdetermined (N unknowns, less than N equations), or overdetermined (more than N equations in N unknowns, none of which are a linear combinations of any others). Such a system can be inverted against observations using standard linear algebraic techniques, such as the method of linear least squares. This method is extremely widely used because of its simplicity and effectiveness.

The problem of inversion is relatively easy to state (if not always to carry out). It simply requires minimising some error function expressing the difference between modelled and observed reflectance values. Consequently, the first task in inverting a model of any sort, linear or non-linear, is to define a suitable error measure describing the difference between model values and measurements, which in practice contain noise of some sort. In least squares estimation, the assumption is made that random measurements of $\rho_i$ are described by a Gaussian (normal) distribution. This assumption is supported by the Central Limit Theorem, which states that in the limit as N approaches infinity, the distribution of the means of N (independent) samples taken from any distribution approaches a Gaussian irrespective of the shape of the original distribution. This assumes that errors are equally distributed between positive and negative. In the absence of any other evidence a Gaussian is the most reasonable choice of probability distribution for a random variable. If no assumption is made about model variance, inverting a CR model is then a question of minimising the sum of the squared errors minimising $e^2$ (familiar least squares) i.e.

$$e^2 = \sum_{i=1}^{N} w_i \left[ \rho_{i,\text{observed}} - \rho_{i,\text{modelled}} \right]^2$$

2.11
i = 1, 2 ... N is the number of observations and w; the associated weights attributed to each observation. The aim is therefore, to find values for which $e^2$ is a minimum, potentially by finding partial derivatives of $e^2$ with respect to parameter weights.

### 2.4.1 Linear inversion

The least squares method is often used in cases where the data are not necessarily normally distributed, but may not differ too far from the Gaussian assumption because of its simplicity and ease of implementation. It is not infallible however. Application of least squares to a bimodal distribution, for example, will result in a solution located between the two modes, where in reality there is only a very small probability of occurrence. Gershenfeld (1999) notes that the square of the difference between the modelled and measured values is not the only power that can be used: if the errors are distributed exponentially, the first power (the magnitude) is the maximum likelihood estimate; higher powers place more emphasis on outliers.

The next stage of model inversion is to obtain estimates of the parameters for the distribution that minimises equation 2.11. In the case of linear models, standard linear algebraic techniques can be applied. In this case, it is assumed the data can be described by a linear summation of M model parameters, $f_j$ i.e.

$$
\rho = \sum_{j=1}^{M} f_j k_j
$$

2.12

$f_j$ are the associated weights of each term. The task is then to find the $f_j$ that minimise the sum of the squared errors between the model values, and a set of N observations $\rho_n$. This problem can be expressed in the form

$$
\begin{bmatrix}
k_1 & k_2 & \cdots & k_M \\
k_1 & k_2 & \cdots & k_M \\
\vdots & \vdots & \ddots & \vdots \\
k_1 & k_2 & \cdots & k_M
\end{bmatrix}
\begin{bmatrix}
f_1 \\
f_2 \\
\vdots \\
f_N
\end{bmatrix}
=
\begin{bmatrix}
\rho_{\text{obs},1} \\
\rho_{\text{obs},2} \\
\vdots \\
\rho_{\text{obs},N}
\end{bmatrix}
$$

2.13

or, more concisely $Gm = d$ (Twomey, 1977). In order to invert a generic linear model of this sort against observed values of reflectance and determine values of $f_j$ that minimise 2.11, a covariance-variance matrix of the model parameters, $k_{MN}$, is formed by multiplying $G$ by its transverse, $G'$. The variance-covariance matrix is then inverted, to give $[G'G]^{-1}$. Multiplying $[G'G]^{-1}$ by $d$ then yields $m$, the vector of $f_j$ values.
If the number of model parameters, $M$, is two or three, the variance-covariance matrix is trivial (and very quick) to invert. This is one reason why linear models have been favoured for many applications, as will be seen in later chapters. For larger order matrices however, inversion is not so simple. However, a variety of methods for performing this task exist, including various elimination and decomposition methods. Press et al. (1994) provide a readable and practical summary of some of these methods, as well as potential pitfalls of implementation and application. One such pitfall is deciding whether a particular system is over- or underdetermined. This is trivial for small systems (only a few model parameters and/or observations), but is not for systems where $M$ and/or $N$ are large. Further, very small changes in the numerical values of some coefficients can rapidly disturb the system from a determined to an underdetermined or indeterminate (contradictory) state. This can cause problems in real systems where measurements always contain noise and the model itself is a series of approximations. The power of linear methods is such that inversion of non-linear systems involving integral transforms is often reduced to linear systems for ease of handling via techniques such as numerical quadrature (Twomey, 1977).

### 2.4.2 Numerical inversion

If the model under consideration is non-linear, and an analytical solution is not generally available (as is most often the case), then further numerical techniques are available to allow inversion of the model (Press et al., 1994; Gershenfeld, 1999). Such techniques can be complex, require a great deal of computational time and may prove to be a limiting factor on the effective application of a particular model. However there are enough techniques that are sufficiently robust and efficient for them to be in common use for inverting non-linear CR models. The following section briefly introduces some of these techniques. The reader is directed to Press et al. (1994) and Gershenfeld (1999) for detailed and extremely readable texts on linear and non-linear model fitting methods.

The basis of numerical inversion of a CR model is the same as that described previously for linear inversion i.e. the formulation of an error metric describing the 'goodness-of-fit' of modelled reflectances compared with observed reflectances (Goel, 1988; Pinty and Verstraete, 1990; Kimes et al., 2000). The problem is then to find the minimum of the error function, which is an optimisation problem (minimisation in this
Optimisation problems are common in many fields, and as a consequence many tried and tested methods exist for their solution. Root mean square error (RMSE) is typically used as the error measure because of the assumption of normally distributed errors (equal probability of positive and negative errors), as in the linear least squares approach (Pinty and Verstraete, 1991). This is an optimal choice if no prior information regarding the form of the error distribution is available. However, it should be noted that this is not the only option (Tarantola, 1987). Numerical inversion is an iterative procedure and generally proceeds in the manner shown in figure 2.5.

Inversion of a CR model against reflectance data is a constrained minimisation problem where some variables lie between fixed limits and cannot take on arbitrary (physically impossible) values. A solution resulting in physically unrealisable parameter values is not valid (or useful). In practice, parameter values should be constrained to lie within physically realisable limits during inversion (this is discussed in greater detail in appendix 1). This is not simply a case of clamping parameters to boundary values when the boundaries are reached, as this equates to arbitrarily moving the location of the current solution on the N-dimensional error surface. Rather, the parameters should remain free but the penalty function (RMSE) should be heavily increased in some way (e.g. exponentially) as the solution heads out of bounds. In this way, subsequent iterations are ‘encouraged’ to move back in bounds by virtue of preferential (lower) RMSE (Press et al., 1994).

All methods of optimisation are prone to the twin difficulties of avoiding local minima and knowing when to stop. Many optimisation methods, gradient methods in particular, tend to ‘fall’ straight down (local) minimum closest to where they started, rather than finding the global error minimum. Unless the characteristic length scale of the problem is known, this is likely to be the outcome. Knowing when to stop can also be difficult, and will depend on the accuracy required: better solutions require a great deal more work for successively smaller improvements. It is also important not to continue past the point where such ‘improvements’ are smaller than the floating-point precision of the machine on which the calculations are being performed (Press et al., 1994).
2.4.3 Multidimensional minimisation

A range of multidimensional minimisation methods have been developed for solving optimisation problems of all types (Press et al., 1994) and many of these have been applied to CR model inversion (Kimes et al., 2000). Although they have mostly been developed for non-linear inversion problems, the distinction is now becoming blurred. As will be seen later, complex non-linear problems can often be well represented by much simpler linear approximations. Hence inversion becomes a hybrid process of linear and non-linear forward and inverse methods, depending on the speed and accuracy required for a particular application.

Some methods are based in the mathematical and computational theory of optimisation, including gradient (Acton, 1990) and simplex methods (Nelder and Mead, 1965; Press et al., 1994). Algorithms requiring well-behaved, continuously differentiable error surfaces have generally been avoided as the error surfaces were not well-understood. Recent work however shows that such surfaces may actually be rather predictable (O'Dwyer, 1999; Barnsley et al., 2001) and this knowledge may be used to restrict parameter space during model inversion.

Other optimisation methods exist which are based on observation of natural systems, which can solve immensely complex optimisation problems in simple and elegant ways. Simulated annealing mimics the thermodynamic properties of cooling crystalline solids (Press et al., 1994), and is particularly suited to problems with error surfaces having many small local minima. Genetic Algorithms (GAs) seek to emulate the slow, incremental improvements of evolution via natural selection (Goldberg, 1998). Artificial Neural Networks (ANNs) approximate the ability of biological neural networks (i.e. brains) to solve complex optimisation problems (Pierce et al., 1994). This is achieved by "training" an ANN to respond according to previously experienced situations, and adapting these responses to new situations. There are a number of examples of the application of ANNs to the problem of inverting biophysical parameters from optical and microwave data of vegetation canopies (Chuah, 1993; Jin and Liu, 1997; Abuelgasim et al., 1996, 1998; Kimes et al., 1997, 2000; Bicheron et al., 1999; Gong et al., 1999). ANNs have also proved very promising for the classification of EO data, where supervised methods (requiring training data) are already the norm (Foody, 1997).
Knowledge-based systems (KBS) comprise a variety of methods which use ancillary data to constrain the parameter space of the optimisation problem (Kimes et al., 2000). An example is the work of Kimes and Harrison (1990) and Kimes et al. (1991) who developed a KBS incorporating spectral (directional) data with a priori information derived from literature, field data etc., into a system for inferring physical and biological surface properties from reflectance data. More recently, Strugnell and Lucht (2000) have demonstrated the use of BRDF ‘archetypes’ (broad classes of BRDF shape) to constrain inversion of BRDF models in the derivation of albedo. The justification is that within classes, the BRDF shapes of different canopies are likely to differ much more in terms of magnitude than shape. Between classes, shape is likely to be more important. This idea of “magnitude inversion” is currently being used in the production of MODIS land surface albedo product for pixels where unconstrained inversion is not possible e.g. through lack of samples of directional reflectance.

Look-up tables (LUTs) are potentially a more promising approach for CR model inversion than either ANNs (limited by training data) or KBS (potentially limited by the ability to describe ancillary data) (Kimes et al., 2000). The LUT approach is to separate the calculation of CR from the problem of finding the optimum solution (model parameter set) to a specific model inversion. An arbitrarily detailed set of discrete CR scenarios can be pre-computed with an arbitrarily complex model and the corresponding parameter values are then stored in the LUT. The optimisation task is then to find the required parameter values in the LUT as quickly as possible, given a set of measured reflectance data (Kimes et al., 2000). Knowledge of external parameters e.g. biome and cover type, viewing/illumination geometry etc. are used to limit the search space as far as possible. Closest matching parameters are then pulled out of the LUT yielding the inverted model parameter set. An important advantage of the LUT approach is that the majority of the computational load i.e. the repeated running of the forward model, is done prior to parameter retrieval and is therefore not a run-time operation. (Running et al., 1996; Kimes et al., 2000). In addition, as developments and improvements are made to the underlying CR model, the LUT can be recomputed and updated accordingly. Knyazikhin et al. (1998a, b) have developed a LUT algorithm for the retrieval of canopy parameters such as LAI and fAPAR from MISR data. O'Dwyer (1999) and Barnsley et al. (2000) examined the use of a LUT in the inversion of the widely-used CR model of Kuusk (1991). Simple grids of CR values of varying densities (two, three or four model parameters) were generated using the Kuusk model (Nilson and Kuusk, 1989) in forward
mode. They showed that in the region of the grid closest to the required solution, the error surfaces are likely to be smooth and well-behaved. As a result, the best solution can be found very rapidly by piecewise linear interpolation between the closest values in the grid. Barnsley et al. (2000) showed that in many cases the error surfaces are simple enough for coarse LUT grids of the order of 4 or 5 steps on a side to be employed, in conjunction with localized linearisation, with no significant loss of accuracy in inversion. Weiss et al. (2000) have also shown the effectiveness of LUT-based parameter retrieval, using (thresholded) average parameter values to interpolate between LUT grid points. In a further development, Combal et al. (2001) have shown that the use of prior information (e.g. ancillary biophysical and architectural measurements) can significantly improve the accuracy of biophysical parameter retrieval through LUT inversion of CR models.

2.4.4 Summary

Figure 2.6 Three extreme types of error surface that may be encountered in function optimisation (after Gershenfeld, 1999).

The preceding section gives a brief overview of some of the numerical methods available for optimisation in CR model inversion. Gershenfeld (1999) illustrates the difficulty of selecting between these methods by subdividing all minimisation problems into three extreme categories (figure 2.6). Each category lends itself to a different type of search. Smooth functions with a single well-defined global minimum are well-suited to gradient searches. Functions with many equally good nearby minima, but no global one, are suited to search by stochastic methods such as simulated annealing and GAs. The third case is characterised by many small local minima, and one clearly defined global minima, requiring some kind of global search method such as ANNs or LUTs. Paradoxically, large minimisation problems are often relatively simple to solve by virtue of having many possible solutions of nearly equal merit: finding one of these from any given starting point is not hard. Small problems are not hard either, as their size permits exhaustive search of the available solutions. Approaching the mid-point of these two size
extremes from either direction however the system becomes too large to search exhaustively, yet not large enough for many good solutions to be obvious. This emphasises the importance of considering the nature of the model, the starting parameter values, and, most importantly, the error function being searched. Information regarding any of these may dramatically improve the search regardless of which algorithm is used.

Of all the methods discussed in the preceding section, LUT-based inversion using localised linearisation appears to be the most promising recent development for improved retrieval of biophysical variables from measured reflectance. This is a result of their highly attractive properties: separation of the major computational load from the operational stage; independence from specific models of CR; rapidity of inversion due to the possibilities for coarse parameterisation; easy incorporation of ancillary data. Much of the experimental work in this thesis is concerned with the application and inversion of linear models of BRDF. However, the distinction between linear and non-linear methods is becoming blurred with the increasing use of LUT methods. Arbitrarily complex non-linear models can be used for populating the search space of canopy reflectance values. However, the search through parameter space during inversion can often be reduced to a linear problem, particularly if the parameter space can be constrained and/or something is known of the error surface itself.
2.5 Canopy reflectance modelling

Canopy reflectance, $\rho_{\text{canopy}}$, is known to be sensitive to a number of factors. These can be broadly divided into two categories:

i. **structural** i.e. the number, angular and spatial distribution of scattering elements.

ii. **radiometric** i.e. the scattering properties of individual canopy elements.

Vegetation components such as leaves and stems are radiometrically characterised by their reflectance ($\rho$) and transmittance ($\tau$) (Jacquemoud and Baret, 1990). A complete canopy, on the other hand, is an aggregation of individual scattering objects. The total $\rho_{\text{canopy}}$ depends on the nature of this aggregation, described by structural properties such as the area density, as well as the angular and spatial distribution (clumping) of scattering elements within the canopy (Ross, 1981; Qin and Liang, 2000). In addition to being a function of canopy (and atmospheric) parameters $\rho_{\text{canopy}}$ will also be a function of the lower boundary beneath the canopy e.g. soil, snow, leaf litter etc. This boundary has its own radiometric and structural properties (microscopic and macroscopic roughness) which may contribute to the measured reflectance signal (Price, 1990; Hapke, 1993). Cierniewski (1987, 1999) and Cierniewski and Verbrugghe (1997) discuss impact of soil roughness on surface BRDF, particularly in relation to large aggregated scattering objects and their resultant shadowing. Nolin and Liang (2000) review recent developments in modelling the BRDF of particulate media, such as soil and snow.

Mathematical models of numerous forms have been developed in order to describe the scattering of radiation from vegetation canopies (Ross, 1981; Goel, 1988; Myneni et al., 1989; Pinty and Verstraete, 1992; Strahler, 1994; Goel and Thompson, 2000). Models have been derived from sources including radiative transfer theory (Ross, 1975), planetary astronomy (Hapke, 1981) and many other areas of mathematics and engineering (Asrar, 1989). The diversity of influences on CR modelling may be regarded as one of the strengths of the field – the ability to adapt methods that have been developed and tested for a whole range of other applications. Approaches to CR modelling can be broadly divided into four categories described in sections 2.5.1 to 2.5.4 (Goel and Reynolds, 1989; Goel, 1992; Strahler, 1994). The following sections briefly describe some of the many modelling approaches, in particular their usefulness for derivation of biophysical parameter information from reflectance data.
2.5.1 Empirical models

Empirical models attempt to describe surface scattering by fitting some (usually simple polynomial) function to observed reflectance data i.e.

$$\rho = F(p)$$  \hspace{1cm} 2.14

where $F(p)$ is some arbitrary function not related to physical properties of the system under observation (Minnaert, 1941; Walthall et al., 1985). The advantages of this approach are firstly that no assumptions are made regarding the type of canopy under observation i.e. whether it is largely homogeneous (e.g. grassland) or more spatially discrete (e.g. tree crowns in a forest canopy). Secondly, the chosen function can be arbitrarily complex in order to describe the surface reflectance behaviour to a desired degree of accuracy. In practice, functions are selected that remain simple enough to invert rapidly. The huge disadvantage of the empirical approach is that there is no physical basis linking the physical scattering behaviour of the canopy and the model coefficients. As a result, purely empirical models tend to be useful for correction/normalisation of directional effects in multi-angular reflectance data, but are of little use for deriving biophysical information (Roujean et al., 1992; Cihlar et al., 1994).

The simplest description of scattering from a surface is that credited to Lambert (Wolff et al., 1992). All radiation incident on a Lambertian surface is reflected equally in all directions. In this case, the Lambert reflectance $\rho_L$ (recall figure 2.1) can be defined as (Hapke, 1981):

$$\rho_L = E_i \cos \theta_i \frac{\cos \theta_i}{\pi}$$  \hspace{1cm} 2.15

$E_i$ is the incident irradiance. The $\cos \theta_i$ term accounts for the reduced component of illumination incident on the surface with increasing illumination zenith angle $\theta_i$, a consequence of the reduced surface area projected in the illumination direction. Reflectance from a Lambertian surface is therefore perfectly diffuse. Minnaert (1941) proposed a simple two parameter empirical model to describe observed brightness variations across the lunar surface. Reflectance is expressed as a function of $\theta_v$ and $\theta_i$

$$\rho = \frac{c(\cos \theta_v \cos \theta_i)^k}{\cos \theta_i} = c(\cos \theta_v)^k (\cos \theta_i)^{k-1}$$  \hspace{1cm} 2.16
where \(c\) and \(k\) are empirical constants. The model thus relates observed reflectance to purely photometric principles, and not to the nature of the observed surface. Hapke (1981) demonstrated that Minnaert's model appears to describe some surfaces well at a limited range of angles, but also points out that both \(c\) and \(k\) themselves are empirical functions of the scattering phase angle and are thus not strictly constants at all. The Helmholtz (H) reciprocity condition is also satisfied by Minnaert's model i.e. the system appears the same if the viewing and illumination vectors are exchanged (Clarke and Parry, 1985). It should be noted that source/detector (S/D) reciprocity (which should not be confused with true H reciprocity) is violated in certain practical cases, particularly when considering reflectance at varying scales. This does not necessarily invalidate model assumptions or conservation of energy arguments (Li and Wan, 1998; Snyder, 1998; Chen et al., 2000).

Walthall et al. (1985) proposed an empirical model more directly suited to describing \(\rho_{\text{canopy}}\), and outlined applications such as describing directional soil reflectance as the boundary condition in a more complex CR model, or as a tool for studying directional effects in multi-angle reflectance data. BRDF is expressed as

\[
\rho = a \theta_v^2 + b \theta_v \cos(\phi_v - \phi_s) + c
\]

\(\phi_v\) and \(\phi_s\) are the view and solar azimuth angles respectively; \(a\), \(b\) and \(c\) are constants to be determined empirically. Walthall et al. (1985) justify the model form by noting that the \(\theta_v^2\) term describes the general upward 'bowl' shape of observed reflectance. \(\rho_{\text{canopy}}\) generally increases with \(\theta_v\) due to the reduced amount of shadowed canopy viewed at these angles (Ross, 1981; Goel, 1988). Figure 2.7 illustrates this. The \(\cos(\phi_v - \phi_s)\) term provides a linear dependence of \(\rho\) on \(\theta_v\), which can account for observed anisotropy in surface reflectance i.e. increased reflectance in the back-scattering direction. The final constant \(c\) can be thought of as a 'brightness magnitude' term. Walthall et al. (1985) demonstrated the ability of their model to accurately fit a variety of measured BRDFs. Due to its simplicity and robustness the Walthall model has been applied in many cases (Barnsley et al., 1997; Privette et al., 1997; Lewis et al., 1999a). As a linear model of three parameters it can also be simply and rapidly inverted. Walthall et al. (1985) updated their model with a fourth term to take account of \(\theta_s\), the sun position, although the model was not reciprocitous. Nilsen and Kuusk (1989) modified the Walthall model to satisfy reciprocity, although this is not strictly necessary in BRDF applications (Chen et al., 2000; Leroy 2001). The updated expression is as follows.
\[ \rho = a + b \theta_v \theta_i \cos(\phi_v - \phi_i) + c \theta_v^2 \theta_i^2 + d(\theta_v^2 + \theta_i^2) \] 2.18

This expression has been used extensively for both the correction of angular effects (Barnsley et al., 1997b; Wanner et al., 1997) and to represent directional soil reflectance as a lower boundary for more sophisticated CR models (Nilson and Kuusk, 1989). Huete (1989) reviews methods of modelling the soil contribution to remote sensing measurements of soil-canopy spectra.

**Figure 2.7** Canopy geometry contributing to BRDF (after Norman et al., 1985). A sees the brightly lit top of leaf 2 and bottom of leaf 1, and very little of the shadowed regions. B sees much more of the shadowed top of leaf 1 and much less of brightly lit leaf 2. As a consequence, the scene appears much brighter to viewer A than viewer B due only to the canopy geometry.

Empirical CR models may represent \( \rho_{\text{canopy}} \) well simply by their generic nature, but their domain of applicability is bounded by the limits of the measurements from which they were derived. A BRDF model may be required to extrapolate to angles beyond those from which the observations are taken (Wanner et al., 1995), or to describe reflectance of canopy types not used in the model derivation. Empirical models are not strictly valid in this case. The largest drawback of empirical models for use in remote sensing of vegetation however is the lack of physical meaning in the model parameters. If biophysical information is required, then physically meaningful relationships between \( \rho_{\text{canopy}} \) and model parameters must be found (Asrar et al., 1989).
2.5.2 Physically-based models

A great deal of effort has been devoted to development of physically-based models of surface scattering (e.g. Suits, 1972; Ross, 1981; Hapke, 1981, 1993; Goel, 1988; Myneni et al., 1988a, 1989). A primary advantage of using physical models is that they are based on physical processes and so their parameters will have some physical meaning. It is also often possible to make reasonable \textit{a priori} estimations of the model parameters, and to constrain them to physically realistic values during inversion. The following section presents a brief overview of various approaches to physically-based CR modelling. Concepts that will reoccur in later chapters are introduced, particularly in regard to simplifications of radiative transfer (RT) and geometric optic (GO) models of reflectance. Goel (1988, 1992) provides a comprehensive review of the theoretical basis of many of these methods (updated by Goel and Thompson, 2000). Qin and Liang (2000) review recent developments in RT modelling techniques, while Chen et al. (2000) do the same for GO modelling.

Strahler (1994) proposes that BRDF is a function of three distinct scattering processes:

1. Coherent superposition of scattered incident radiation. This can cause a retro-reflectance peak (hotspot), but is dependent on the mean free path between scattering events within the canopy being of the order of the wavelength of the incident radiation. Coherence is generally ignored for vegetation, but is important for soils (Hapke, 1984, 1993).

2. Scattering effects resulting from the arrangement of objects on the surface i.e. specular reflectance, and reflectance variations caused GO shadowing assuming parallel rays of incident radiation (Otterman and Weiss (1984), Li and Strahler (1985, 1986) for vegetation; Ranson and Daughtry (1987) for shrubs and snow; Cierniewski (1987) for soil). The scale of these effects ranges from microscopic roughness, to shadowing due to topography (Liang et al., 2000a).

3. Volume (diffuse) scattering behaviour of aggregated canopy elements. This is particularly important for dense vegetation and is modelled using RT methods, based on the work of Chandrasekhar (1960). As higher orders of photon scattering are considered, the interactions become increasingly random in direction, and the volume scattering component tends to become isotropic.
In a complex physical system such as that of photon interaction with vegetation, often the only effective way to achieve a manageable\(^1\) and tractable representation of the system is to make approximations. Typical requirements of a physical CR model are:

- To represent (selected/all) scattering features of the canopy in the spatial, spectral and angular domains.
- Agreement with \(\rho_{\text{canopy}}\) measurements of a real canopy of the same type to a specified accuracy (according to some criterion such as RMSE).
- To relate observed reflectance behaviour to the controlling biophysical parameters sufficiently well such that these parameters may be derived from measured reflectances through model inversion.
- To allow generalisations of theoretical treatments of canopy scattering based on observed scattering behaviour.

The following section describes some of the approaches that have been taken to simplify the physical approach to CR modelling, and highlights the diversity of models which have been developed for a huge variety of cases.

2.5.2.1 Canopy reflectance, the turbid medium and radiative transfer (RT)

One of the most powerful tools used in modelling canopy scattering behaviour is that of radiative transfer. RT theory was developed by Chandrasekhar (1960) as a method describing radiation transport in the gaseous clouds formed during stellar evolution. Chandrasekhar's idea has since been modified and applied in many fields, including canopy reflectance modelling. In this approach the canopy is approximated as a layer (or layers) of infinitely extended, plane-parallel homogenous scattering medium consisting of randomly oriented infinitesimal scattering phytoelements ('leaves'). This so-called 'turbid medium' approach is illustrated in figure 2.8. The assumption of the canopy as a turbid medium allows a number of approximations and simplifications to be made regarding canopy scattering behaviour (Goel, 1988; Myneni \textit{et al.}, 1989; Pinty and Verstraete, 1998).

\(^1\) Manageable implies the problem can be represented to an acceptable accuracy, and is not prohibitively computationally expensive.
Figure 2.8 Schematic representation of the turbid medium approximation, showing the various scattered components of exitant radiation.

The turbid medium approach has proved a powerful technique modelling photon transport in vegetation canopies and has been applied widely to the problem (Ross, 1981; Goel and Strebel, 1984; Myneni et al., 1988a,b; Myneni et al., 1989; Qin and Liang, 2000). The radiance field resulting from single and multiple scattered photon interactions (see figure 2.8) can be described by considering the conservation of energy within each canopy layer, and specifying the sources of radiation external to that layer (boundary conditions). The result is an integro-differential equation describing the change in intensity along a viewing direction $\Omega$ due to i) scattering interactions causing radiation to be scattered out of the illumination direction $\Omega'$ (sink term), and ii) interactions causing radiation to be scattered from other directions into the direction $\Omega$ (source term). If the so-called far-field approximation is made (Myneni et al., 1990), whereby scattering elements are assumed to be infinitesimal and there is no mutual shadowing (and polarization, frequency shifting interactions and emission are disregarded) the problem of upward and downward energy fluxes within the canopy can then be represented as a solution of the well-known radiative transfer equation (Chandrasekhar, 1953) i.e.

$$-\mu \frac{\partial l(z, \Omega)}{\partial z} + \sigma_s(z, \Omega) l(z, \Omega) - \int_{\Omega} \sigma_s(z, \Omega' \rightarrow \Omega) l(z, \Omega') d\Omega' = 0$$

$\mu l(z, \Omega)$ is the specific energy intensity at a height $z$ within a horizontal plane-parallel canopy of total height $T$ ($0 < z < T$) (so $\partial l(z, \Omega)/\partial z$ is the steady-state radiance
distribution function); \( \sigma_e \) is the extinction coefficient of the canopy medium; \( \sigma_s \) is the differential scattering coefficient for photon scattering from direction the illumination direction \( \Omega' \) into a unit solid angle about the viewing direction \( \Omega \).

This problem has been studied extensively in astrophysics, planetary astronomy, particle physics and neutron transport among other fields, and many methods are available for its solution under certain conditions (Chandrasekhar, 1960). To solve equation 2.19 for a vegetation canopy, approximations regarding \( \sigma_e \) and \( \sigma_s \) are often made (Shultis and Myneni, 1988; Goel, 1988; Ross and Marshak, 1989; Myneni et al., 1989, 1990, 1995b). Other approaches attempt to include modifications for observed features such as the hotspot (Nilson and Kuusk, 1989; Gerstl and Borel, 1992). Perhaps the most difficult problem in solving equation 2.19 is that of modelling the source term, as this requires keeping a 'scattering history' of each photon from one interaction to the next (Myneni et al., 1991). This problem is to all intents and purposes insoluble analytically (Knyazikhin et al., 1992), but approximations can be made (Myneni and Ganapol, 1991) or a computer simulation model can be used (see section 2.5.3). It is also necessary to define the boundary conditions in the case of a canopy illuminated from above. At the top of the canopy the incident radiation can be considered to consist of diffuse and direct components of solar irradiation. In addition, some radiation arriving at the base of the canopy re-radiates isotropically back up through the canopy effectively creating a source function at the lower canopy boundary (Knyazikhin and Marshak, 2000).

Modified forms of equation 2.19 have been the basis for many detailed investigations into \( \rho_{canopy} \) (Gerstl and Zardecki, 1985; Goel and Grier, 1988; Shultis and Myneni, 1988; Ahmad and Deering, 1992; Rahman et al., 1993a,b; Iaquinta and Pinty, 1994; Liang and Strahler, 1993b, 1994; Knyazikhin and Marshak, 2000). Further approximations and simplifications have been applied for specific types of canopy (e.g. Goel and Grier, 1988 for row crops). A variety of numerical techniques have been applied to solving RT in a vegetation canopy, including Successive Orders of Scattering Approximation (SOSA) (Myneni et al., 1987a), Gauss-Seidel methods and discrete ordinates (Shultis and Myneni, 1988; Myneni et al., 1988a). Perhaps the most widely-used simplification however, has been to treat single and multiple scattering interactions separately. A brief outline of these methods is given below.
2.5.2.2 Approximations made possible by the turbid medium approach

One of the most powerful approximations used in modelling reflectance behaviour is to concentrate on single scattering interactions within the canopy. Single scattering interactions are in most cases the dominant component of $\mu_{\text{canopy}}$ (Myneni et al., 1989; Myneni and Ross, 1990), particularly at visible wavelengths. Considering single scattering interactions within a turbid medium, the radiation intensity in the incident direction, $\Omega'$, at a depth $z$ within the canopy can be described using Beer's law (Beer-Lambert law) (Monsi and Saeki, 1953):

$$ I(\Omega', z) = I(\Omega', 0) \exp \left( -\frac{L(z)G(\Omega')}{\mu'} \right) $$  \hspace{1cm} 2.20

$I(\Omega', 0)$ is the direct irradiance incident on the top of the canopy; $L(z)$ is the downward cumulative LAI in the canopy at depth $z$ (m$^2$m$^{-3}$). This is actually $u(z)$, the leaf area density (one-sided leaf area per unit volume of canopy at depth $z$ in the canopy in m$^2$m$^{-3}$) integrated over all $z$. $G(\Omega')$ is the leaf projection function i.e. the fraction of leaf area projected in the illumination direction $\Omega'$; $\mu'$ is the cosine of the illumination zenith angle, $\theta_i$. $G(\Omega)$, the leaf projection function (in the viewing direction), is defined as

$$ G(\Omega) = \frac{1}{\pi} \int_{\Omega_i} g_s(\Omega_i) \Omega_i \cdot \Omega d\Omega_i $$  \hspace{1cm} 2.21

g_s(\Omega_i) is the angular distribution of the leaf normals, $\Omega_i$ i.e. LAD. $g_s(\Omega_i)$ is typically assumed to be spherical for simplicity i.e. all leaf orientations are equally probable (Myneni et al., 1988a, 1990). Although this is a widely used assumption, it can cause inaccuracies (Kimes, 1984; Goel and Strebel, 1984; Verstraete, 1987).

Beer's law as stated is for a perfectly homogeneous canopy, and the LAI parameter takes no account of the possibility of vegetation being clumped. This is highly unlikely in practice (Ross, 1981). If LAI is redefined as effective LAI, $\text{L}_{\text{e}}$, then a true LAI can be defined as $L = \text{L}_{\text{e}}/C$, where $C$ is a clumping index (Ross, 1981; Nilson and Kuusk, 1989). If $C > 1$ then leaves are regularly dispersed within the canopy e.g. row crops; if $C = 1$ then leaves are dispersed randomly; if $C < 1$ then the canopy is clumped dense patches of vegetation interspersed with voids (gaps between the clumps). As clumping increases, $\text{L}_{\text{e}}$ decreases, and the probability of gaps in the canopy increases leading to a higher soil reflectance for given LAI.
The assumption of the turbid medium, along with the approximations required to derive Beer’s law, permits a description of the single scattering radiance field within a vegetation canopy as a function of a small number of simple structural parameters. A normalised leaf scattering phase function, $\Gamma(\Omega' \rightarrow \Omega)$, describing the angular distribution of scattering (from the illumination direction $\Omega'$ into the viewing direction, $\Omega$) at each photon interaction (c.f. $\sigma_i$ in equation 2.19) and a joint gap probability, $Q(\Omega' \rightarrow \Omega, z)$, can be derived (Ross, 1981). $Q$ describes the probability of existence of free lines of sight to the top of the canopy for a photon travelling from $\Omega'$ to $\Omega$ at a depth $z$ within the canopy. Clearly, if a photon is unable to make it both down and back up to the top of the canopy, it will not emerge to be available for measurement (without further scattering). If the far-field approximation is made, then $Q(\Omega' \rightarrow \Omega, z)$ is simply the probability of photons travelling a distance $z/\mu'$ in direction $\Omega'$, multiplied by the probability of travelling $z/\mu$ in the direction $\Omega$. The individual gap probabilities in the downward and upward paths can be calculated according to Beer’s law (equation 2.20).

The far-field approximation applies when scattering elements are small enough not to interfere with the joint gap probability, such as in neutron transport or cloud physics (Chandrasekhar, 1960; Dickinson, 1983). However this is not the case in a vegetation canopy where scattering elements have a finite size (Myneni et al., 1989; Myneni and Asrar, 1993). Further approximations are required to circumvent this problem (Myneni and Ganapol, 1991; Myneni et al., 1991; Knyazikhin et al., 1992; Pinty and Verstraete, 1998). Single scattered $\rho\text{canopy}$ can then be expressed as a sum of the single scattered contributions from vegetation and soil, $\rho^s\text{soil}$ and $\rho^s\text{vegetation}$. $\rho^s\text{soil}$ is simply the probability of a photon penetrating to the base of the canopy ($z = 0$) and escaping again, multiplied by the soil reflectance. Using Beer’s law

$$\rho^s\text{soil}(\Omega', \Omega) = Q(\Omega' \rightarrow \Omega, z)\rho^s_\tau(\Omega', \Omega)$$  \hspace{1cm} \text{(2.22)}$$

$\rho^s\text{vegetation}$ can be shown to be (Ross, 1981)

$$\rho^s\text{vegetation}(\Omega', \Omega) = \frac{\Gamma(\Omega' \rightarrow \Omega) + G(\Omega')\mu + G(\Omega)\mu'}{G(\Omega')\mu + G(\Omega)\mu'} \left[ 1 - \exp\left( - \frac{L G(\Omega')\mu + G(\Omega)\mu'}{\mu\mu'} \right) \right]$$  \hspace{1cm} \text{(2.23)}$$

Thus single scattering $\rho\text{canopy}$ is a function of both structural (LAI, $g(\Omega_i)$) and radiometric parameters (leaf and soil reflectance, leaf transmittance, $\tau_{\text{leaf}}$). $G(\Omega_i)$ requires the evaluation of an integral (equation 2.21) so any attempt to find an analytical solution
for equation 2.23 requires approximations regarding $g(\Omega)$ to be made. Many models simply assume a spherical LAD (Goel, 1988) i.e. all leaf angles are equally likely, in which case $g(\Omega)$ is 1 and $G(\Omega)$ is 0.5 (Asrar et al., 1989; Myneni et al., 1989). Other approaches include the discrete geometrical distribution of Bunnik (1978) based on observed data; the continuous two-parameter beta distribution of Goel and Strebel (1984); the elliptical distribution of Nilson and Kuusk (1989), controlled by mean leaf angle and eccentricity parameters.

Equation 2.19 can be further simplified if the assumption is made that $\rho_{\text{leaf}}$ and $\tau_{\text{leaf}}$ can be considered Lambertian (bi-Lambertian) and equal (i.e. $\rho_{\text{leaf}} = \tau_{\text{leaf}}$) (Ross, 1981). In this case, single scattered canopy reflectance, $\rho_{\text{canopy}}$ can be described as

$$
\rho_{\text{canopy}} = \frac{4\rho_{\text{leaf}}}{3\pi} \left[ \frac{\sin \gamma + \cos \gamma \left( \frac{\pi}{2} - \gamma \right)}{\mu + \mu'} \right] \left[ 1 - \exp \left( \frac{-L \mu + \mu'}{2 \mu \mu'} \right) \right] + \rho_{\text{soil}} \exp \left( \frac{-L \mu + \mu'}{2 \mu \mu'} \right)
$$

where $\gamma$ is the phase angle between $\theta_i$ and $\theta_r$. This relatively simple analytical expression has been widely used in practice (Wanner et al., 1995, 1997) and forms the basis of some of the semi-empirical models described in section 2.5.4, which are the basis of much of this thesis.

Many models have been based on the approach outlined above (Goel, 1988), originating from the work of Monsi and Saeki (1953). The major assumption underpinning Beer’s law is that the number of scattering objects in a volume of canopy (leaves, stems etc.) is proportional to its volume. However, Knyazikhin et al. (1998c) show that the structure of vegetation canopies may in some cases be fractal in nature, resulting in non-linear relationships between canopy volume and the density of scattering elements. They suggest that modifications may need to be made to extend the applicability of Beer’s law in such cases. However, it has been shown that the basic formulation of Beer’s law can be a useful tool in describing single scattering interactions within the canopy (Monsi and Saeki, 1953).

Approximations based on the turbid medium approach have been widely applied to describing $\rho_{\text{canopy}}$. Although single scattering interactions dominate $\rho_{\text{canopy}}$ at visible wavelengths (typically 95% of total reflectance), the multiple scattered component of $\rho_{\text{canopy}}$ becomes important if scattering in the near-IR region is considered (up to 50% of
total reflectance). As a result, approximations to the multiple scattering component of $\rho_{\text{canopy}}$ have also been developed (although the multiple scattered component may be important in magnitude, it is less so in terms of BRDF as a result of the tendency of multiple scattered radiation to be scattered in all directions). Descriptions of multiple scattering are typically based on simplifications of and approximations to the RT equation (equation 2.19), some of which are described briefly below. The remainder of this thesis concentrates on consideration of the single scattering component of $\rho_{\text{canopy}}$ so a detailed description of the many formulations for canopy multiple scattering approximations is not given here. Myneni et al. (1989) and Qin and Liang (2000) review these methods in detail.

2.5.2.3 Limitations of the turbid medium approach

A major drawback of the turbid medium approach is that the size of the scattering objects within the canopy is not considered. By definition, the canopy is assumed to be a homogeneous medium of infinitesimal scatterers (to satisfy the far-field approximation) with mutual shadowing not permitted. Consequently, expressions describing the reflected radiation from such a canopy do not contain information regarding the size of scattering objects (Qin and Liang, 2000). However, certain properties of observed $\rho_{\text{canopy}}$, particularly the hotspot, are directly controlled by the size and orientation of scattering objects (Kuusk, 1985; Hapke, 1986; Marshak, 1989; Jupp and Strahler, 1991; Pinty and Verstraete, 1998). Turbid medium approximations will not capture such features, and if the size of scattering objects is to be considered a different approach is needed. Myneni et al. (1991) considered voids between finite dimensional canopy elements in order to model the dimensions of scattering elements explicitly. Their model represents the hotspot feature quite accurately and gives far better agreement of scattered reflectance in the hotspot direction than treatments than those which ignore scatterer size.

In a series of excellent papers discussing the theory of diffuse scattering from particulate media, Hapke (1981, [and Wells] 1981, 1984, 1986) developed a comprehensive model of bidirectional reflectance from the RT theory of Chandrasekhar (1960) for use in planetary astronomy. Hapke constructed an analytic expression describing the bidirectional reflectance from a particulate surface, formulating analytic expressions for (amongst other things) single scattering albedo, integral phase function...
and bihemispherical radiance. The importance of Hapke’s approach is the analytical nature of his model, and the inclusion of a hotspot term. Hapke’s approach has been successfully applied, with modifications, to modelling $\rho_{\text{canopy}}$ (Verstraete et al., 1990; Pinty and Verstraete, 1991; Iaquinta and Pinty, 1994). Single and multiple scattering are treated separately with the single scattered radiation being characterised exactly and the multiple scattered radiation being approximated using a two-stream approach. This can cause errors however, because of the greatly increased multiple scattering occurring in the near-IR wavelength region (Liang and Strahler, 1994) as described above. Others have proposed a more exact four-stream approximation for the solution of multiple scattered radiation (e.g. Liang and Strahler, 1995). Some of the earliest developments in CR modelling used the two-stream approximation in order to describe the radiation field in a canopy. Suits (1972) used a four-stream approximation to calculate radiation intensity from the projected horizontal and vertical canopy scattering elements. This approach was extended by Verhoef (1984) to handle arbitrary leaf angles in the widely-used Scattering by Arbitrarily Inclined Leaves (SAIL) model.

Separation of canopy fluxes into uncollided and collided intensities of various orders (Kubelka and Munk, 1931; Suits, 1972; Hapke, 1981) has often been employed in order to simplify the RT approach (Myneni et al., 1990; Verstraete et al., 1990; Iaquinta and Pinty, 1994; Gobron et al., 1997). The discrete properties of the canopy (those related to the size and distribution of scatterers) tend to impact only the first few orders of scattering. As the scattering order increases, these features tend to become ‘smeared out’ by the multiple scattering interactions (Marshak, 1989; Liang and Strahler, 1993a; Iaquinta and Pinty, 1994). Dividing the radiation field into collided and uncollided intensities as opposed to following a standard RT treatment may preserve these features. Hapke’s original theory has been extended, notably Verstraete et al. (1990), Dickinson et al. (1990) and Iaquinta and Pinty (1994), to overcome the inability to account for finite sized scattering elements. Ahmad and Deering (1992) added a specular reflection term to Hapke’s empirical hotspot term, resulting in a relatively straightforward analytical model which agreed well with various measured reflectance data. But the number of model parameters (8) and the coupling between them limits the use of the model for inversion of biophysical information.

The above discussion illustrates how the behaviour of a real vegetation canopy is likely to diverge rapidly from classical RT theory as a result of finite leaf size (Myneni
and Ganapol, 1991). As the canopy becomes denser, mutual shadowing cannot be ignored (Myneni et al., 1991; Myneni and Asrar, 1993). It also becomes increasingly difficult to justify using convenient values of scattering phase function, leaf normal distribution and leaf projection function based on the assumption that leaf normals are randomly oriented and azimuthally invariant. This is clearly partially or wholly violated for a number of canopies, particularly row-oriented agricultural crops. Verstraete et al. (1990) proposed replacing the components of the full RT treatment explicitly dependent on leaf size and orientation (e.g. \( \sigma_s \) and \( \sigma_c \), which are impossible to characterise exactly for a large canopy of many leaves) with a parameterised average description. However, accounting for the discrete nature of vegetation within a RT (continuous) description of the canopy radiation regime leads to an apparent paradox (Knyazikhin et al., 1998c): the more accurate the representation of canopy geometry, the less accurate the description of radiation transport and photosynthesis in the canopy is likely to be. Knyazikhin et al. (1998c) use a fractal description of a plant stand at scales at which the assumptions underlying the RT approach break down (i.e. at leaf level) to demonstrate the difficulty of scaling the RT approach from leaf to canopy scale.

Once the size of scattering elements in the canopy is considered, gaps between the scatterers must also be considered. Myneni and co-workers have developed a model based on considering the canopy as a binary medium of convoluted voids (gaps between leaves) only broken by the leaves themselves (Myneni et al., 1991). Further problems are caused by the fact that the diffuse component of illumination impinging on the canopy will itself contain a component of radiation reflected back from the top of the canopy (Knyazikhin and Marshak, 2000). A number of authors have considered this problem, and various coupled surface-atmosphere scattering models have been developed (Rahman et al., 1993a,b; Liang and Strahler, 1994). These models can significantly improve agreement between measured and modelled reflectances, at the expense of model complexity. Solution of the RT equation in a vegetation canopy is still a complex problem, however, despite all approximations. As a result, inversion of such models must also be performed numerically, or using LUTs. Additionally, the approximations made in order to formulate equation 2.29 result in the driving parameters of such models being relatively far-removed from parameters directly representative of physical canopy properties.
2.5.2.4 Geometric-optic (GO) models

In direct contrast to the turbid medium approach, GO models of $\rho_{\text{canopy}}$ describe surface scattering due to discrete objects (spheroids, blocks, cylinders etc.) arranged on a surface under the assumption of parallel-ray geometry. This approach is exemplified by the work of Li and Strahler (1985, 1986, 1988, 1992) in a series of papers investigating the use of cones and spheroids to model the scene variance of forest canopies. Their work extended that of Egbert (1976), and Otterman and Weiss (1984) who were able to explain a significant proportion of the measured reflectance of soybean using a model composed of thin, vertical cylindrical protrusions. Significantly, they concluded that while retrieving the reflectance of the cylinders through inversion of the model might be possible, retrieval of the projected shadow (effectively the cylinder size) would not.

Li and Strahler postulated that a typical forest canopy comprises large, discrete crowns of a variety of shapes, separated by relatively large intervening spaces. They considered simple geometric objects (cones) with a lognormal height distribution and known number density located randomly on a Lambertian plane. The resulting areal proportions of sunlit and shadowed canopy and soil components were then calculated using GO theory. This is illustrated in figure 2.9. The scene geometry is controlled by $r$, the cone base radius; $\alpha$ - half the crown apex angle; $h$, the crown height; $\gamma$ is the angle identifying the portion of the cone illuminated beyond the cone half ($\sin^{-1}(\tan\alpha/\tan\theta)$). Scene reflectance is divided into four components: sunlit crown, sunlit ground, shadowed crown and shadowed ground. The geometry of a particular scene is calculated according...
the size and density distribution of objects, and the average reflectance of a scene pixel is then a linear sum of the various areal proportions i.e.

$$S = \frac{(A_G G + A_C C + A_Z Z + A_T T)}{A}$$

(A_G, A_C, A_Z, A_T) are the areas of illuminated background and crown, and shadowed background and crown respectively; G, C, Z, T are the multispectral reflectance vectors for unit areas of illuminated background and crown, and shadowed background and crown respectively. Variations in S are caused by variations in crown density and size in each pixel. Initially the model was formulated for non-overlapping cones, but a general case based on the theory of the moments of overlapping areas has been developed (Li and Strahler, 1992). Ciemiewski (1987, 1999) followed a similar approach in formulating a model of soil reflectance by calculating the shadowing of a square grid of equally sized spheres on an arbitrarily inclined plane.

![Diagram of spheroid-on-a-stick](image)

**Figure 2.10** (left) Geometry of spheroid-on-a-stick with shape controlling parameters and shadowed area A(θ) (right) nadir (a) and off-nadir (b) areas of illuminated shadow (A_C, A_T, A_Z, A_G = as in figure 2.9) (after Strahler and Jupp, 1990).

Strahler and Jupp (1990) extended the GO approach, using Boolean models of random set overlap to model the BRDF of forest and woodland as a collection of randomly located ‘spheroids on sticks’. This is illustrated in figure 2.10. The spheroids, with major and minor axes b and r respectively, are located a height h above the surface (the concept of the stick is merely to indicate height above the surface). The nadir and off-nadir illumination and shadow components of the scene are also shown. The model treats the areal proportions of sunlit and shadowed components at both the scene level and the leaf level, resulting in a two-stage model. Chen and Leblanc (1997) have examined
the application of GO modelling at scales larger and smaller than tree crowns, and in particular the impact of the departure from the Lambertian assumption with varying scale.

The GO approach has been further developed by consideration of a vegetation canopy as a collection of scattering elements located within a GO "envelope". Scattering within the envelope can be handled using some model of attenuation (e.g. Beer’s law, or a full RT approach), whilst shadowing at canopy stand-level is modelled using the standard GO theory discussed above. This hybrid GO-RT approach (Li et al., 1994, 1995) relies on the calculation of gap probabilities between crowns and the path lengths within crowns (Li and Strahler, 1988). Roujean et al. (1992) follow a similar line to that of Li et al. (1994) by combining non-overlapping opaque blocks randomly located on a Lambertian surface modelled using GO theory, with an RT description of the attenuation within the blocks. Goel and Grier (1988) modelled reflectance of inhomogeneous canopies by combining the GO and RT approaches with some success. In a similar way, Bégué (1992) models the directional reflectance of regular-clumped canopies by considering (radiometrically) porous cylinders located on a hexagonal grid. This hybrid approach combines the benefits of the GO approach i.e. the inherent ability to describe the discrete nature of a discontinuous canopy (shadowing, hotspot, crown size etc.), with the RT approach to scattering within the crown envelopes (accurate description of radiation interception and multiple scattering). For this reason both GO and RT models are considered in the semi-empirical approach described in section 2.5.4.

2.5.3 Computer simulation models

To solve the RT problem of photon scattering in a homogeneous medium, approximations regarding the size, orientation and spatial distribution of scatterers within the canopy are required. An ideal solution would specify these properties in 3D for every scattering element in the canopy in order that the behaviour of every photon could be modelled physically. This implies an enormous number of parameters controlling \( p_{\text{canopy}} \) making it impossible to invert such a model directly. However, with increases in computing power and memory it is possible to construct physically detailed 3D models which can be run in the forward mode. The results of these models can then be used to test the assumptions and approximations that are made in the physically based models described above (Govaerts, 1996; Kuusk et al., 1997; Disney and Lewis, 1998), or to
populate LUTs for indirect inversion algorithms (Kimes et al., 2000). There are two primary methods for implementing "scene simulation" models, ray tracing (based on a Markov chains) and radiosity (originating from thermal engineering). Both these methods have benefited (particularly in terms of practical implementation) from developments in computer graphics (CG) (Goel, 1988; Goel and Thompson, 2000).

2.5.3.1 Ray Tracing

Ray tracing is a method of rendering realistic images of 3D scene representations through detailed modelling of scene illumination and shading (Foley et al., 1992). Ray tracing essentially involves calculating the intersections of rays (photons) “fired” into a 3D scene with the objects in the scene, and determining the behaviour of the photons at each intersection. The subsequent direction and energy of a scattered photon following an intersection is governed by the radiometric properties of absorption, transmission and reflection of the surface at the point of intersection in addition to the geometric scattering properties (phase function) of the object. Objects are not limited to representation by simple polygons. Volumetric objects (treating scattering through radiative transfer) can be used, in conjunction with a description of the (volumetric) scattering properties of the materials contained within (North, 1996). Shadows can be simulated by the casting of ‘shadow’ rays from objects to the light source and diffuse sampling can also be used to simulate diffuse light sources (Govaerts, 1996; Lewis, 1999). Realistic depiction of the bidirectional reflectance of any scene (represented as a collection of 3D objects) can be simulated by repeating the sampling process for every sample (pixel) in the viewing plane (Disney et al., 2000).

Ray tracing is computationally expensive compared to $\rho_{\text{canopy}}$ models based on RT or GO approaches. Every object within a scene must be represented accurately in 3D along with associated radiometric properties, and this information must be stored in memory. Intersection tests are carried out for each fired ray to see where (if at all) they intersect the scene, and for each subsequent interaction (and for shadowing). In addition, to achieve a convergent solution (representing the scattering behaviour of the scene to within some accuracy threshold) some form of numerical integration, typically Monte Carlo sampling (Press et al., 1994; Veach, 1997) is used. Clearly, the more detailed the scene, the more calculations are required for each photon. Objects within the scene are
composed of polygonal or volumetric primitives, and the primitives can be chosen to be of arbitrary size – larger for coarser representation but quicker calculation and lower storage requirements; smaller for finer detail, but requiring more processing and storage. A range of variance reduction techniques and CG methods, such as the use of bounding-boxes, can be used to further speed up the ray tracing process (Disney et al., 2000).

A variety of implementations of ray tracing have been developed for remote sensing scene simulation. Ross and Marshak (1988) developed a simple model for radiometric scene simulation. Goel et al. (1991) demonstrated ray tracing for simulating reflectance of corn plants. The model of Govaerts (1996) has been used for comparison with a variety of RT modelling techniques (Govaerts et al., 1995; Gobron et al., 1997) and target BRDFs. Govaerts (1996) and Lewis (1999) have used ray tracing to simulate the timed-return signal of LiDAR (Light Detection and Ranging) instruments, which are an interesting new development for probing vegetation canopy structure (Dubayah et al., 1997). Chelle and Andrieu (1999) have used ray tracing to validate a physically-based CR model (Kuusk et al. 1997). North (1996) developed a ray tracing model to simulate GO $\rho_{\text{canopy}}$ in forest stands (Gerard and North, 1997), as well as for simulation of synthetic Along-Track Scanning Radiometer (ATSR-2) data. The BRDF modelling community has recently initiated an ongoing model intercomparison exercise, RAMI (RAradiation Transfer Model Intercomparison, Pinty et al., 2001 and www[2.2]). The aim of the exercise is to establish the strengths and weaknesses of BRDF models of all types, in a carefully controlled model “bake off”. The ongoing RAMI exercise has shown that ray tracing models are the most flexible, if slower than other types of model. The trade off is that they can simulate almost any conceivable canopy configuration and hence can be used to benchmark more approximate models.

### 2.5.3.2 Radiosity

Radiosity methods originated in thermal engineering and have been adapted for realistic scene simulation techniques in computer graphics (Goral et al., 1984). In contrast to the view/illumination oriented approach of ray tracing (all calculations based on a particular viewing/illumination configuration), radiosity is based solely on the scene geometry. All energy emitted or reflected by every surface in a scene is accounted for by its reflection and absorption by other surfaces (Foley et al., 1992). The rate at which
energy leaves a surface (the radiosity) is then simply the sum of the rates at which the surface emits energy and reflects or transmits it from other surfaces. To calculate BRDF, all light interactions in an environment are calculated independent of view (the so-called 'view' or 'form factors' of each surface). Scene radiosity can be calculated very simply for an arbitrary view. Radiosity is even more computationally expensive than ray tracing when the view factors are being calculated, but this need only be carried out once for any particular scene/illumination scenario (the two methods reduce to essentially the same solution calculated in different ways under certain conditions). Borel et al. (1991) show that radiosity methods can be used to simulate scenes for use in analysis of remotely sensed data. They apply the radiosity method to modelling a layered plant canopy, and draw parallels between the radiosity and RT solutions. Qin and Gerstl (2000) have coupled 3D plant models (derived from L-systems) with radiosity to simulate reflectance of semi-arid scrubland. Their results agree well with field, and provide further proof that explicit 3D plant modelling in combination with radiosity or ray tracing methods can be extremely useful in scene simulation at a range of scales.

### 2.5.3.3 Other numerical CR modelling methods

Another interesting numerical approach is that adopted by Gastellu-Etchegorry et al. (1996) in their DART (Discrete Anisotropic Radiative Transfer) model, which is some way between ray tracing and radiosity. Based on the 3D canopy transport model of Kimes and Kirchner (1982) DART simulates RT in heterogeneous 3D scenes that may contain many elements. A scene is simulated as a 3D matrix of parallelepipedic cells (voxels), and the phase functions of each cell are calculated from the scattering behaviour of the elements contained within the cell. DART significantly extends the Kimes and Kirchner model as it can cope with non-uniform, unequally spaced cells, and multiple scattering processes within cells. The microwave model of Sun and Ranson (1995) is functionally similar to that of Gastellu-Etchegorry et al. (1996) in that a solution is formed over 3D gridded (voxel) space. This raises the prospect of coupled microwave and optical models of canopy response based on 3D structural canopy representations. This appears to be a realistic and sensible goal in that in both cases, the models are designed to describe the physical interaction of light with matter; the difference is only one of wavelength of the incident radiation. This approach might also be extended to a third domain: thermal wavelengths.
The major advantage of the explicit 3D representation of geometry required for ray tracing and radiosity is that every object within a canopy can be represented to whatever level of detail is required or is convenient. Ray tracing is ideally suited for precisely modelling the scattering processes used in RT techniques as leaves and voids in the canopy are modelled explicitly. Assumptions that are made in such models regarding the size and orientation distribution of scattering elements within a canopy can also be modelled explicitly. Clearly this type of complex numerical model cannot be inverted directly but such models can be very useful for testing the approximations made in other (invertible) scattering models designed. Further, the development of LUT methods make it increasingly feasible to invert biophysical information from such models, albeit indirectly.

2.5.3.4 BPMS/ararat model

Simulation of $\rho_{\text{canopy}}$ used in chapters 4-7 of this thesis is undertaken using the 3D model of Lewis (1999). This forms part of the Botanical Plant Modelling System (BPMS) (Lewis and Muller, 1990; Lewis, 1996, 1999) which has been used for simulating canopy radiation for a wide range of purposes (Lewis, 1996; Lewis and Disney, 1997, 1998; Disney et al., 2000). The BPMS essentially consists of software tools and protocols and for capturing, representing and processing 3D data representing the canopy-soil system; Ararat (the Advanced Radiometric Ray Tracer) is a Monte Carlo ray tracing tool for simulating the radiation regime within the 3D canopy.

3D canopy architecture can be specified within the model in a number of ways e.g. from photogrammetric measurements, or through the use of growth rules, such as a modified L-systems approach (Prusinkiewicz and Lindenmayer, 1990; Prusinkiewicz, 1999). L-systems have proved eminently suitable for the development of 3D plant and canopy models (de Reffye et al., 1988; de Reffye and Houllier, 1997; Prusinkiewicz, 1999). 3D representations of individual plants can be constructed within the BPMS from manual measurements of a few key structural parameters, such as leaf and stem lengths and widths, leaf base and tip zenith and azimuth angles etc. These properties are extrapolated (using specified functional relationships) to a full 3D representation of individual plants (surfaces are tessellated with polygons, triangles by default, during ray
tracing). Individual plants can then be ‘cloned’ (duplicated with arbitrary rotation and translation) and then ‘planted’ on a surface according to some predefined pattern to build up a full canopy.

The ray tracing part of the BPMS (ARARAT, the Advanced RAdiometric RAy Tracer) is also very flexible, having been designed specifically for investigating scattering in plant canopies. Information can be stored as a function of scattering order within a simulated scene, permitting analysis of multiple scattering (Lewis and Disney, 1998). Arbitrary camera models can be used (e.g. allowing integration over the entire viewing hemisphere in order to directly simulate albedo), as can texture mapping, material mapping and diffuse sampling. Associated information such as the proportions of sunlit and shadowed canopy components can also be calculated (Lewis, 1999). The BPMS can incorporate ancillary data in addition to measured plant parameter data, such as row and plant spacing, seed depth, digital elevation models (DEMs) of the underlying soil surface etc. This flexibility make the BPMS an extremely useful tool for examining BRDF model operation (Lewis and Disney, 1997, 1998; Disney and Lewis, 1998) as well as more general properties such as spatial variation of $\rho_{canopy}$ (Lewis et al., 1999b).

The experiments described in chapters 4-6 use values of $\rho_{canopy}$ simulated from 3D plant data measured in the field, processed via the BPMS plant modelling software, and rendered by the ray tracing component, ararat. The BPMS/Ararat model was chosen because of its flexibility as well as the capability for analysing canopy radiation as a function of canopy parameters. Several other models are used in the experimental chapters of this thesis, and these are listed below with an explanation of where and why they are used, as well as indications as to where more detailed descriptions of each model can be found.
Table 2.1 Canopy reflectance models used in this thesis.

<table>
<thead>
<tr>
<th>Model</th>
<th>Used</th>
<th>Reason</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPMS/ararat</td>
<td>Chapters 4-6</td>
<td>Flexibility: can represent full 3D structure at arbitrary scale, and simulate radiation under arbitrary viewing and illumination conditions.</td>
<td>Canopy simulation carried out using Monte Carlo ray tracing, in reverse mode (rays traced from viewer back to illumination source), with importance sampling at each ray intersection. More details in Lewis (1996, 1999).</td>
</tr>
<tr>
<td>Linear kernel-drive</td>
<td>Referred to and/or used in chapters 4-7.</td>
<td>Basis of thesis: models are currently in use generating MODIS albedo product. Assumptions underlying these models are tested using BPMS/Ararat model.</td>
<td>Simple semi-empirical, kernel-driven models, based on more complex physical models of BRDF. Described in detail in section 2.5.4</td>
</tr>
</tbody>
</table>

2.5.4 Semi-empirical models

The final class of CR models to be mentioned are semi-empirical (so-called kernel-driven) models. These have been developed in response to the requirement for dynamic (near real-time) estimates of global albedo (Wanner et al., 1995; Lucht et al., 1999; Lucht and Roujean, 2000). Generation of albedo in near real-time from the large quantities of moderate resolution (hundreds of m to km scale) data from instruments such as MODIS and MISR requires rapidly invertible models capable of describing reflectance from spatially heterogeneous scenes at sub-km resolution (Roujean and Leroy, 1992; Wanner et al., 1997).

Semiempirical models attempt to bridge the gap between the physical and empirical modelling approaches (Wanner et al., 1995). The aim is to maintain some physical basis, while still allowing rapid analytical inversion against moderate resolution
data. The assumption is made that at moderate resolution, scattering from heterogeneous surfaces will be composed of separable scattering components (kernels). Each kernel represents a particular component of canopy scattering behaviour, and contributes to the overall reflectance 'shape'. Approaches using either linear additive or multiplicative combinations of kernels have been developed (Lucht and Roujean, 2000). Linear kernel-driven models assume reflectance is composed of volumetric and GO scattering components. Multiplicative models are based on magnitude, anisotropy and hot-spot terms. Both approaches are less flexible for describing BRDF than purely empirical models. This is because they are constrained to the basic shapes represented by individual kernels. A benefit of this constraint however, is that it permits extrapolation as well as interpolation, which is not the case for purely empirical models.

2.5.4.1 Linear (kernel-driven) semi-empirical models

Linear semi-empirical models assume that scattering from homogeneous surfaces can be described using a weighted linear superposition of a small number of kernels based on approximations to physical solutions for volumetric and GO scattering. The general form of the linear kernel-driven models is (Wanner et al., 1995)

$$BRDF(\theta_i, \theta_v, \phi, \lambda) = \sum_n f_n(\lambda) k_n(\theta_i, \theta_v, \phi; \{P_n\})$$

Where the $k_n$ kernels are purely geometrical expressions of fundamental scattering behaviour of radiation within the canopy; $f_n$ are the model parameters, and $P_n$ are potential preset terms that may modify the kernels behaviour. More specifically, BRDF is typically considered as

$$BRDF(\theta_i, \theta_v, \phi, \lambda) = f_{iso}(\lambda) + f_{vol}(\lambda) k_{vol}(\theta_i, \theta_v, \phi) + f_{GO}(\lambda) k_{GO}(\theta_i, \theta_v, \phi)$$

$k_{vol,GO}$ are the kernels representing volumetric and GO scattering components of BRDF ($k_{iso}$ is assumed to be unity); $f_{iso,vol,GO}$ are the spectrally dependent model parameters (weights associated with each kernel). Importantly, the kernels depend only on $(\theta_i, \theta_v, \phi)$ and hence can be pre-calculated for angular integration. Although approximate in nature, the physical basis of the various kernels can be used to provide meaningful constraint of the model inversion process (see appendix 1), as well as (potentially) providing
biophysical information, as will be seen in later chapters. Semiempirical models require more samples than purely physical models, but far less than purely empirical ones.

Describing BRDF as a linear superposition of volumetric and GO BRDF ‘shapes’ is justified by considering that any moderate resolution pixel will contain surfaces contributing both volumetric and GO scattering to the total pixel reflectance. This is modulated by the respective sub-pixel areas (weights) of each cover type (Wanner et al., 1995). Even for scenes likely to be dominated by a single type of scattering there will probably be some contribution from the other component. Wanner et al. (1995) use the example of a forest canopy, where reflectance from the discrete crowns is likely to be characterised largely by GO scattering. However, the dense vegetation within the crowns is likely to contribute some component of volumetric scattering to the total BRDF. This does assume that there is no multiple scattering between the separate components. The kernels are based on the assumption of single-scattering interactions only and to compensate for this multiple scattering is included in the isotropic term. Scattered radiation from a directional source tends to become increasingly isotropic with successively higher order scattering interactions. Hence it seems reasonable to include multiple scattering (as a first approximation) as an additive (scaling) "brightness" term, rather than as a function of viewing or illumination angle. In the linear kernel-driven models the isotropic term is defined as the nadir reflectance at nadir illumination.

There are several major advantages of the linear kernel-driven approach to modelling BRDF.

1. Being linear, the models lend themselves to rapid, analytical inversion using methods described previously (Lewis, 1995).
2. As the forms of the kernels are known in advance, angular integrals of BRDF directional-hemispherical and bihemispherical reflectance ($\bar{\rho}$ and $\bar{\rho}$) can be pre-calculated in a LUT. Total albedo can then be calculated as a weighted sum of the kernel albedos, avoiding computationally expensive numerical integration (Wanner et al., 1997).
3. Most importantly, if adjacency effects over heterogeneous regions are neglected (Wanner et al., 1997), the linear models can be assumed to scale linearly with area. They can therefore be arbitrarily scaled for application to any required resolution, making them ideal for production of albedo at a range
of scales. The linear scaling property also means that such models can be applied to surfaces with arbitrary combinations of volumetric and GO scattering with no requirement for a priori assumptions of cover type.

4. Finally, as the model parameters have some physical basis there is the hope that parameter estimates might be inverted to provide biophysical information.

Due to the approximate nature of the kernels it is not straightforward to determine what information is contained within the inverted model parameters, or how this might be exploited (Disney and Lewis, 1998). The remainder of this thesis is concerned with examining what type of biophysical information may be derived from reflectance data using kernel-driven models, and how such models might be improved. The derivation of the kernels is presented below.

2.5.4.1.1 Volumetric kernels

A number of kernels approximating volumetric and GO scattering have been developed. The volumetric kernels are based on Ross' (1981) solution for RT in a turbid medium. Two separate versions of the so-called Ross kernel for canopies with LAI >> 1 (RossThick) and LAI << 1 (RossThin) are described below. The RossThick kernel was developed by Roujean et al. (1992), from Ross's formulation for BRDF given in equation 2.24, assuming: a horizontally homogeneous canopy (randomly oriented leaves) over a flat Lambertian surface of reflectance $\rho_o$; single scattering only; leaf reflectance ($\rho_{\text{leaf}}$) = leaf transmittance ($\tau_{\text{leaf}}$). The assumption is then made that LAI >> 1, in which case LAI dominates the $\exp(-\text{LAI} \cdot \sec\theta_i + \sec\theta_v)$ terms. The $\sqrt{\sec\theta_i + \sec\theta_v}$ terms (denoted B) are replaced with a typical value over the angle range $\theta_i, \theta_v = 0^\circ, 30^\circ, 60^\circ$ of 1.5. In this case, $R_{\text{thick}} = c_1k_{\text{vol}} + c_2$ and the RossThick kernel is

$$k_{\text{vol(thick)}}(\text{RossThick}) = \frac{(\xi - \tilde{\xi}) \cos \tilde{\xi} + \sin \tilde{\xi}}{\cos \theta_i + \cos \theta_v} - \frac{\pi}{4}$$

\(\xi\) is the phase angle of scattering, and $\cos \tilde{\xi} = \cos \theta_i \cos \theta_v + \sin \theta_i \sin \theta_v \cos \phi$. The $\pi/4$ term arises from a convention introduced by Roujean et al. (1992) that the kernels should satisfy the condition that $k_{\text{vol}} = 0$ when $\theta_i, \theta_v = 0$. The constants $c_1$ and $c_2$ are $c_1 = \frac{4\rho_{\text{leaf}}}{3\pi} \left(1 - e^{-\text{LAI}}\right)$ and $c_2 = \frac{s}{3} + e^{-\text{LAI}} \left(\rho_o - \frac{\rho_{\text{leaf}}}{3}\right)$ respectively. $c_1$ is the weight of
the kernel in the full kernel-driven model (equation 2.27) and $c_2$ is included in the isotropic term.

The adaptation of the Ross volumetric kernel for LAI $\ll 1$ has been proposed by Wanner et al. (1995). In this case the approximation that $e^x \approx 1 + x$ if $x$ is small is made. If $R_{\text{thin}} = c_1 k_{\text{thin}} + c_2$, the RossThin kernel for volumetric scattering (from equation 2.24) is

$$k_{\text{vol}}(\text{RossThin}) = \frac{(\xi - \zeta) \cos \zeta + \sin \zeta}{\cos \theta_i \cos \theta_v} - \frac{\pi}{2} \tag{2.29}$$

where this time, the constants $c_1 = \frac{2 \rho_{\text{leaf}} \text{LAI}}{3\pi}$ and $c_2 = \frac{\rho_{\text{leaf}} \text{LAI}}{3} + \rho_i$. In the same way as for the RossThick kernel, $c_1$ is the weighting of the kernel in the full linear model, and $c_2$ is included in the isotropic brightness term. Both kernels are functions of $\theta_i$ and $\theta_v$ only, as desired.

### 2.5.4.1.2 GO kernels

The GO kernels are based on the work of Li and Strahler (1986), described above and Roujean et al. (1992). Shadowed regions are assumed perfectly black (no contribution to scene reflectance) and sunlit crown and ground components are assumed equally bright. Wanner et al. (1995) consider the proportions of sunlit crown and ground resulting from spheroidal protrusions of length 2$b$ and width 2$r$, number density $\lambda$, randomly located at height $h$ above a flat Lambertian surface (c.f. fig. 2.10). To calculate the area of projected shadow, the spheroids are transformed to the ‘equivalent’ sphere that would result in the same shadowed area at given $\theta_i$, $\theta_v$. The resulting (transformed) zenith angles are denoted $\theta'_{\iota}, \theta'_{\nu} = \tan^{-1}(b/r \tan \theta_{\iota,\nu})$. Two GO kernels are presented; one for scenes in which mutual shadowing of spheroids is not permitted (LiSparse), and one for the mutual shadowing case (LiDense). In the same manner as for the volumetric kernels, reflectance is expressed as $R_{\text{GO}} = c_1 k_{\text{sparse}} + c_2$, and the LiSparse kernel is

$$k_{\text{GO}}(\text{LiSparse}) = O(\theta'_{\iota}, \theta'_{\nu}) - \sec \theta'_{\iota} - \sec \theta'_{\nu} + \frac{1}{2} (1 + \cos \xi') \sec \theta'_{\nu} \tag{2.30}$$

$$\cos \xi' = \cos \theta_i' \cos \theta_v' + \sin \theta_i' \sin \theta_v' \cos \phi'.$$ $O(\theta'_{\iota}, \theta'_{\nu}, \phi')$ describes the overlap between the areas of viewing and illumination shadow dependent on the transformed zenith angles, height $h$, and ratio of $b$ to $r$. The constants $c_1$ and $c_2$ in this case are $C\lambda \pi r^2$ and $C$
respectively, where $C$ is the reflectance of the sunlit crown and ground (assumed equal).

This dependence on the size distribution of the spheroids results in a family of kernels for
different $b/r$ and $h/b$. In practice these are reduced to four cases for oblate/prolate
spheroids, and high/low crowns.

The LiDense kernel describes $\rho_{canopy}$ including mutual shadowing by considering
the spheroids on the surface as tree crowns with lognormal height distribution. In this
case, $R_{GO} = c_1 k_{dense} + c_2$ and the LiDense kernel is:

$$k_{GO}(LiDense) = \frac{(1 + \cos \xi') \sec \theta'_v}{\sec \theta'_v + \sec \theta'_v - \mathcal{O}(\theta'_v, \theta'_v)} - 2$$  \hspace{1cm} \text{(2.31)}

The factor of 2 is subtracted to ensure the kernel is zero for $\theta_v, \theta_v = 0^\circ$. All other terms are
as above, except $c_1 = C/2$ and $c_2 = C$. The dependence on the ratios $b/r$ and $h/b$ remain.

Figure 2.11 shows the directional variation of the full complement of Ross and Li kernels.
Included are GC (Ground-Crown) versions of the LiSparse and LiDense kernels. The GC
versions treat the ground and crown as having different brightnesses. The asymmetric
bowl shape is apparent in both the Ross and Li kernels. The peak in the backscatter
direction is present only in the Li kernels as it is a manifestation of the finite size of scattering elements, and hence is not described by the RT approximation. This peak is
more prominent in the LiDense kernel (mutual shadowing of spheroids permitted).

Figure 2.12 shows the family of LiSparse kernels with various values of $h/b$ and
$b/r$, including:

- high oblate (HO) $h/b = 2.5$, $b/r = 0.75$;
- high prolate (HP) $h/b = 2.5$, $b/r = 2.5$;
- low oblate (LO) $h/b = 1.5$, $b/r = 0.75$;
- low prolate (LP) $h/b = 2.5$, $b/r = 2.5$.

Figure 2.13 shows the corresponding family of LiDense kernels. In practice (i.e. in
production of the MODIS nadir reflectance and albedo product) the RossThick LiSparse
kernel combination is used, in preference to RossThin and/or LiSparse. The RossThick
LiSparse combination fits as well or better than any other in most circumstances, and so
has become the de facto choice of linear kernels (Schaaf et al., 2000a).

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Figure 2.11 Angular variation of the Ross and Li kernels.

Figure 2.12 Family of LiSparse GO kernels.
Two other kernels should be mentioned. Firstly, a GO kernel developed by Roujean et al. (1992) based on the sunlit and shadowed scene components due to randomly oriented rectangular Lambertian blocks of height $h$, length $l$ and width $b$ arranged on a surface. Shadows are assumed perfectly black and all sunlit areas are considered equally bright, with reflectance $\rho_o$. Mutual shadowing is ignored, restricting the validity of the model to situations where shadows do not fall outside the basal area of the block casting them (i.e. $\theta_\alpha, \theta_\varphi < 60^\circ$). Additionally $l$ is assumed $>> h$, and $l > b$ in order that the shadowing by the sides of the blocks (area $bh$) may be disregarded. The reflectance of blocks on a surface is expressed as

$$R_{\text{Roujean}} = c_1k_{\text{Roujean}} + c_2$$

where $k_{\text{Roujean}}$ is

$$k_{\text{Roujean}} = \frac{1}{2\pi} \left[ (\pi - \phi) \cos \phi + \sin \phi \right] \tan \theta_\varphi \tan \theta_\alpha - \frac{1}{\pi} \left( \tan \theta_\varphi + \tan \theta_\alpha + \sqrt{\tan^2 \theta_\sigma + \tan^2 \theta_\varphi + 2 \tan \theta_\varphi \tan \theta_\alpha \cos \phi} \right)$$

and $c_1$ and $c_2$ are $\rho_o h/b$ and $\rho_o$ respectively. This has recently been extended to the LiTransit kernel (Gao et al., 2001).

The other kernel included is that of Walthall et al. (1985) described in equation 2.17, and in its modified form in equation 2.18. This expression is also dependent only on
viewing and illumination. In practice, the modified Walthall model often provides a better fit to observed data (in terms of RMSE) than the volumetric or GO kernels (Lucht et al., 1999). However, it suffers from the drawback of all empirical models, namely that inverted model parameters have no physical meaning. Whilst the linear models were developed in order to facilitate production of integrated products such as albedo, there is naturally an interest in their capability for producing biophysical parameter information. However it is not clear to what extent the kernels contain (uncoupled) biophysical information, or how this information might be interpreted. The remainder of this thesis seeks to explore this problem.

Goel and Thompson (2000) note that a limitation of the kernel-driven approach to modelling BRDF is that the assumption that there is little cross coupling between volumetric and GO scattering within a scene may be hard to justify in some cases. They conclude that the sensitivity of the kernels to angular sampling makes it difficult to determine the weightings for different sensor sampling regimes. However Lucht and Lewis (2000) have shown that it is possible to determine in advance the dependence of the kernels on sampling. Knowledge of the sampling characteristics of new sensors (Barnsley et al., 1994) can be used to overcome this dependence (Lucht, 1998).

2.5.4.2 Non-linear semiempirical models

There has been parallel development of non-linear (or semi-linear) semiempirical models (Rahman et al., 1993). In contrast to equation 2.26, non-linear models typically follow the form

$$BRDF(\theta_i, \phi, \lambda) = \prod_n t_n(\theta_i, \phi, \lambda; \{f_n(\lambda)\})$$

2.33

where \(t_n\) are the terms controlling basic scattering shape, and \(f_n\) are the model parameters. Multiplicative kernel-driven models of this sort tend to have complementary benefits and disadvantages over the linear models, and are currently being used to model surface reflectance from MISR data (Martonchik et al., 1998b). The RPV model (Rahman et al., 1993a) is based on Minnaert's empirical function given in equation 2.18, modified to include a Henyey-Greenstein phase function term describing the asymmetry of the BRDF between forward- and backscattering, and a hotspot term. The advantages of this approach are that despite its empirical core, the RPV model has physically meaningful
parameters. In addition, the multiplicative nature of the model means a larger number of BRDF shapes can be represented than with a purely additive model. However, non-linearity implies numerical (or iterative) inversion, which is a major drawback. In practice, a semi-linear modified version of the RPV model (MRPV) (Martonchik et al., 1998b) is used which may be inverted using an iterative LUT-based approach. This forms the basis of surface reflectance retrieval for MISR (Martonchik et al., 1998b). Intercomparison between the best-performing linear and non-linear semiempirical models (RossThick LiSparse and MRPV) has shown their performance to be comparable in most cases, with only marginal differences between them (Lucht, 1998; Lucht et al., 1999).

2.6 Conclusion

The preceding discussion illustrates the huge variety and ingenuity of approaches to CR modelling, as well as some of the benefits and drawbacks in each case. Empirical models are simple, generally fit observed BRDF well and may be useful as directional interpolants. However they require many directional samples to constrain their fit, and are not valid for extrapolation. Physical models require many less samples and have physically meaningful parameters, but are generally complex and require numerical inversion. Computer simulation models can represent canopy scattering at in almost arbitrary detail but are often computationally intensive, and are not invertible directly due to the potentially very large number of controlling parameters. Semiempirical kernel-driven models bridge the gap between simple empirical and complex physical descriptions of BRDF. Kernels describing various scattering properties can be linearly or multiplicatively combined to describe BRDF. Kernel-driven models can be used to interpolate or extrapolate from limited samples of BRDF, and can be rapidly inverted against measured reflectance at arbitrary scales.

The remainder of this thesis is concerned with the ability of the linear semiempirical models to describe BRDF. They are the models of choice for production of global BRDF and albedo products from the MODIS instrument. The ability of the linear models to describe BRDF, even in unfavourable circumstances, is examined, along with novel methods for extracting biophysical information from their parameters.
3 Description of field-measured data

The data used in the experimental chapters of this thesis were collected during the growing season of 1997 from a study site based around Barton Bendish Farm, Norfolk (52° 37.2' N 0° 32.0' E). The farm covers some 9 km² and produces winter wheat, several varieties of spring barley, peas and sugar beet. Due to the initial work done here (Disney et al., 1997) and subsequent field experiments, this site and the surrounding area has been taken on as a MODIS core validation site.

Three barley fields, and one wheat field were selected at the start of the fieldwork campaign. These fields are identified as follows (and will be referred to as such throughout):

<table>
<thead>
<tr>
<th>Date</th>
<th>Fields</th>
</tr>
</thead>
<tbody>
<tr>
<td>barley 24th April</td>
<td>Fields ba_104, ba_112 and ba_119.</td>
</tr>
<tr>
<td>barley 13th May</td>
<td>Combines measurements made from the 13th - 15th May 1997 (due to bad weather) in fields ba_112 and ba_119.</td>
</tr>
<tr>
<td>barley 4th June</td>
<td>Fields ba_104, ba_112 and ba_119</td>
</tr>
<tr>
<td>barley 24th June</td>
<td>Fields ba_112 and ba_119</td>
</tr>
<tr>
<td>wheat 23rd March</td>
<td>Field ww_109</td>
</tr>
<tr>
<td>wheat 23rd April</td>
<td>Field ww_109</td>
</tr>
</tbody>
</table>
Figure 3.1 AVHRR image of UK (top left); SPOT FCC image of East Anglia (top right); aerial photograph of Barton Bendish farm (bottom) showing selected fields used in fieldwork study, August 1997 (courtesy of NERC).
Figure 3.1 shows the fieldwork site at three different scales: an AVHRR image of the UK (9/8/95) showing the East Anglia region; a false-colour composite SPOT image (4/4/97) of the NIR, visible red and green bands highlighting vegetation as red. Also shown is a scanned aerial photograph of the Barton Bendish farm and surrounding area (6/8/97), obtained by the Natural Environmental Research Council (NERC) Airborne Research System (ARS) Facility aircraft. The Barton Bendish farm area and the fields selected for this study are marked on the image. RAF Marham air-base, clearly visible in the SPOT image, is just visible at the top of the aerial photograph. The cereal crops have been harvested at this stage, and the remaining green areas are fields of sugar beet.

It can be seen that there are quite large variations in the soil brightness throughout the site, caused by differences in soil composition and drainage efficiency. To compensate as far as possible for any effect this variability may have on crop density and/or structure, as many samples as possible were taken from within each field. Data were also collected from several fields during each visit to minimise the possibility of selecting an atypical field of any particular crop. The planned temporal sampling (a full set of complementary measurements every two weeks) was not achieved due to the inclemency of the weather during the growing season of 1997. This resulted in a lack of sampling between early May and early June.

3.1 Summary of data, collection methods and validation

The field data, collected on eight visits to the Barton Bendish field site between 24th April and 6th August 1997, consist of measurements of a number of properties including:

- Ground spectro-radiometric measurements.
- Canopy coverage estimates.
- LAI measurements.
- Canopy height, and plant and row spacing.
- 3D plant structure, for BPMS modelling, characterisation of LAD.
- Airborne data (NERC ARS ATM, CASI data and aerial photography).
Data collection methods are described in detail below, in addition to validation studies performed in order to provide confidence in the measured data. This is primarily a comparison of 3D barley and wheat canopies reconstructed from measured plant parameter data using the BPMS, with properties measured in the field such as LAI, LAD and BRDF. The ability to characterise the primary structural properties (and the consequent radiometric behaviour) of the measured canopies within the BPMS is fundamental to this thesis. Much of the following work deals with analysis of BPMS-simulated canopy reflectance. Establishing agreement between reflectance behaviour simulated using measured plant parameters within the BPMS, and the reflectance behaviour of the real canopies, permits conclusions drawn from analysis of BPMS results to be applied to real data. The canopy structural data collected through manual measurement are first described, followed by various other measurements collected for validation of the BPMS data and for subsequent comparison with information derived from airborne data.

How the various sources of data described above are subsequently used within this thesis:

- **3D structural measurements**: described in section 3.1.1, these measurements were used within BPMS/Ararat generate 3D scene representations of barley and wheat canopies. Values of $\rho_{\text{canopy}}$ was simulated under realistic conditions (multiple scattering, direct and diffuse illumination) in order to compare with field-measured reflectance data. This provides independent validation of the 3D modelling approach (described in section 3.1.2). Subsequent simulations of $\rho_{\text{canopy}}$ are performed under the assumptions made in the formulation of the linear kernel-driven models (single scattering only, $\rho_{\text{leaf}} = \tau_{\text{leaf}} = 0.5$, Lambertian soil) in order to investigate these assumptions (chapters 4, 5, and 6).

- **Canopy structural measures**: described in sections 3.1.2 and 3.1.3, properties such as LAI, %cover and canopy directional reflectance were measured directly in order to compare with values derived from canopies generated using the 3D structural measurements within the BPMS.

- **Airborne Thematic Mapper Data**: described briefly in section 3.1.5, these data are used in chapter 7 to test the kernel-driven approach to modelling spectral, directional reflectance (in particular, image of June 6th 1997 is used).
3.1.1 Plant structural measurements

Plant and row spacing for each field were recorded along with the planting densities of the various crops i.e. the number of plants per meter\(^1\). In addition, detailed descriptions of the topology and structure of individual plants were made for use within the BPMS. These measurement techniques are discussed in detail by Lewis and Muller (1990), Lewis and Disney (1997) and Lewis (1999). Typically five or six plants per field per date were measured. A set of ten measurements were made of each plant, with the 'leaf' subset of these measurements being made for every leaf of a plant. Brief details of the measurements are as follows:

For each tiller:
- *tiller azimuth angle*
- *tiller zenith angle*

For each stem section (emergent from ground, and between leaf nodes):
- *stem length*
- *stem width*

For each leaf:
- *leaf base zenith angle*
- *leaf tip zenith angle*
- *leaf length*
- *% leaf length to maximum width*
- *(maximum) leaf width*

---

\(^1\) This does not take account of some areas in the barley and wheat fields where the seed drilling vehicle has crossed back on itself leading to patches of doubly drilled crop. These areas are noticeably denser than the main body of the fields and were avoided for all measurements.
Individual leaf angles (base, tip) and stem section angles were measured with a protractor to an estimated precision of 5°. Leaf length, maximum width and stem lengths were measured to an estimated precision of 1 mm. Figure 3.2 shows a measured barley plant. Sensitivity analysis was carried out to test whether simulated BRDF is sensitive to any particular BPMS measurement. The measured parameters were perturbed randomly according to a Gaussian distribution of specified mean and standard deviation and BRDF was simulated for each 'perturbed' canopy. Simulated BRDF was found to be more sensitive in shape to row and plant spacing than any of the individual structural measurements, and more sensitive in magnitude to the specified leaf and soil reflectance values. Figures 3.3 and 3.4 show simulated canopies using BPMS measurements.

**Figure 3.2** Wireframe representation of manually measured barley plant (13/5/97) showing measured parameters.
Figure 3.3 Simulated wheat canopy in early growth stage, Lambertian soil.

Figure 3.4 Simulated barley canopy (shortly prior to harvest) with Lambertian seed heads and soil properties modelled on observed soil spatial statistics.
3.1.2 Ground spectro-radiometric measurements

Measuring BRDF in the field is not trivial, largely because of variable atmospheric conditions and hence varying quantities of diffuse and direct illumination (Sandmeier and Itten, 1999). Other uncertainties are caused by the difficulty of determining precisely what the instrument IFOV is seeing, movement of crops due to wind, lack of a stable instrument base etc. Although no atmospheric scattering data were available during this field campaign (sun photometer measurements are now made at Barton Bendish to augment field measurements), measurements were recorded rapidly and repeated often to try and minimise the effects of changing atmospheric conditions. In addition, BRDF measurements were restricted to 'blue sky' days. However, these can be few and far between in a typical UK summer and 1997 transpired to be particularly wet. However, samples of directional reflectance were made with a boom-mounted ASD PS-II radiometer (www[3.I]) in the visible to NIR wavelength range (due to limitations in the instrument, effectively, 450-900 nm). Measurements were made at 10° intervals in view zenith (θv) from −70° to +70° in both the principal and cross-principal solar planes2. The relative azimuth angle, φ, between θv and the illumination zenith, θi, is then 0° or 90° for

2 Negative angles in this case imply measurements in the backscatter direction, and positive ones the specular direction.
viewing in or across the principal plane. This viewing and illumination geometry is illustrated in figure 3.5. In addition to the target radiance measurements, near-simultaneous radiance measurements of a polythene (assumed) Lambertian reference panel were made. Reflectance is then calculated as the ratio of the target radiance to that of the reference panel (see equation 2.2). For each reference panel measurement, the so-called dark current response of the instrument was also recorded. This is a measurement of the signal recorded when no light is incident on the radiometer, caused by background (thermal) noise in the silicon detector. The dark current is subtracted from the measured radiance to provide an accurate measurement of target radiance. An example of measured barley BRDF is given in figure 3.6, along with reflectance simulated using the manually measured canopy structural parameters within the BPMS.

![Figure 3.6](image)

**Figure 3.6** Measured and simulated canopy reflectance at four bands (barley field ba_119, 13/5/97, LAI = 3.89; $r_{\text{leaf}}$ and $\tau_{\text{leaf}}$ from laboratory measurements, $\rho_{\text{soil}}$ from field measurements$^3$).

Agreement between the modelled and measured reflectance data is reasonable at visible wavelengths ($r^2 > 0.7$), but not so in the NIR (850nm) ($r^2 < 0.5$). Whilst the

---

$^3$ Laboratory measurements provided by B. Hosgood from LOPEX data set (Hosgood et al., 1994); field measurements provided by E. J. Milton at NERC EPFS facility, Southampton, UK.
directional variation of simulated reflectance may be reasonable, the magnitude is generally too low. This is a result of reflectance being simulated without multiple scattering (as discussed in section 2, the multiple scattered component of canopy reflectance tends to be isotropic, and will therefore increase the magnitude of simulated canopy reflectance without significantly changing the shape). In addition, the level of noise in the measurements can be seen. This is particularly obvious at nadir where three measurements were made, one at the start of the string of measurements, one in the middle and one at the end. The variability of these measurements (up to 10% reflectance) is caused largely by changes in atmospheric conditions during the measurement period, even on a 'blue sky' day with little or no cloud. This is a typical problem when performing field radiometric measurements and is discussed at the end of this chapter, as well as in chapter 8. Values of $r^2$ for linear regression of the measured against modelled reflectances are given in table 3.1.

**Table 3.1** Values of $r^2$ for comparison of measured to modelled reflectances.

<table>
<thead>
<tr>
<th>canopy</th>
<th>450nm</th>
<th>550nm</th>
<th>650nm</th>
<th>850nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ba_112 18/04</td>
<td>0.82</td>
<td>0.84</td>
<td>0.87</td>
<td>0.68</td>
</tr>
<tr>
<td>ba_119 13/05</td>
<td>0.94</td>
<td>0.95</td>
<td>0.89</td>
<td>0.74</td>
</tr>
<tr>
<td>ba_112 04/06</td>
<td>0.90</td>
<td>0.96</td>
<td>0.95</td>
<td>0.80</td>
</tr>
<tr>
<td>ba_119 24/06</td>
<td>0.79</td>
<td>0.84</td>
<td>0.80</td>
<td>0.71</td>
</tr>
<tr>
<td>ww_109 23/03</td>
<td>0.78</td>
<td>0.80</td>
<td>0.78</td>
<td>0.64</td>
</tr>
<tr>
<td>ww_109 23/04</td>
<td>0.92</td>
<td>0.95</td>
<td>0.89</td>
<td>0.83</td>
</tr>
</tbody>
</table>

The figures in table 3.1 demonstrate reasonable between the measured and modelled canopy reflectance values, however there is significant disagreement in a number of cases. The cases where agreement is not so good are likely to be due to the canopy being very sparse (LAI <<1). The agreement between the angular variation is higher than the spectral variation. Overall agreement between the BPMS and measured reflectance values is generally good in the visible but the variance of the NIR reflectance values is clear. The signal-to-noise ratio (SNR) of the detector in the region beyond 900nm (SNR ≈5:1) is very much lower than in the visible part of the spectrum (SNR better than 20:1).
3.1.3 Canopy coverage estimates

Nadir-pointing photographs were taken (from a height of 1m above the ground) of the various canopies throughout their development. No photographs were taken during the later stages when the canopy heights exceed 1m as there was total coverage in these cases. A series of canopy cover photographs showing the progression of cover in barley field 119 are shown in figure 3.8. The variability of local planting density (even in such a small region) is clear in the 13th May image. The camera tripod is visible at the lower extent of the first two images.

Figure 3.8 Canopy cover photographs for barley canopy 119 (from l to r) on 18th April, 15th May and 24th June 1997.
Canopy cover was derived from the photographic data by estimating the proportion of visible soil per unit ground area (Disney et al., 1998). Only the central portion of each image was used to avoid image plane distortions caused by the relatively wide field of view (115°). RGB to HSI transformations were performed on the scanned images, which were then thresholded manually on hue. The mid-range hue values corresponded closely to soil, while the higher values corresponded to vegetation. This allows percent cover to be simply estimated. Values of % cover as estimated from the photography are presented in figure 3.9 in the form of a scatter plot with corresponding BPMS derived values. The error bars in figure 3.9 represent the variability of % cover estimates made from photography (one SD). For the barley, twenty eight separate %cover images were used from four dates; for wheat, ten images from two dates were used. The regression of all samples together shows reasonably high correlation, with a slight offset (overestimation) of around 10% in the values derived from photography. This is due to inaccuracy in the thresholding of the HSI-transformed photography. Relatively small changes in the value of the selected threshold cause significant changes in % cover. Conservative threshold values were chosen deliberately to make sure all vegetation was included.

![Figure 3.9](image.png)

**Figure 3.9** %cover estimated from photography and BPMS simulations.
3.1.4 LAI measurements

LAI measurements were made with a LI-COR LAI 2000 instrument, which works by comparing the intensity of (diffuse) incident illumination measured at the bottom of the canopy with that arriving at the top (LI-COR technical report; Welles and Norman, 1990). Incident light is recorded over five concentric angular rings, each of approximately 15° in width (giving a nearly hemispherical field of view). LAI is estimated by calculating the probability of a photon penetrating to a depth $z$ in the canopy (under various assumptions regarding the arrangement and radiometric properties of scattering elements in the canopy), and comparing this with the measured radiance at the bottom of the canopy. The probability of non-interceptance at depth $z$ within the canopy is described by Beer’s law (equation 2.20). The angular integral of this property (over all zenith angles) is approximated as a weighted summation over the five concentric angular rings of the instrument.

The manufacturer’s recommendations were followed in deciding a measurement plan. One measurement was made at the top of the canopy followed by ten measurements at different locations below the canopy. This pattern was repeated three times per field, and the resulting thirty-three samples comprise one full set of measurements. Measurements were made following transects at an angle of between 30° and 45° to the row direction, and at intervals suitably spaced to avoid over or under-estimation of LAI caused by measuring at integer numbers of rows or inter-row gaps. Care was also taken with regard to the illumination conditions under which measurements were made. The instrument operates under the assumption that the canopy is illuminated by a diffuse source, and therefore should be shadowed from any direct sunlight. Due to the weather during the fieldwork campaign it was possible to make the majority of the measurements under diffuse conditions. On days with significant direct sunlight a 270° view cap was used to mask out both the operator and sun from the viewing hemisphere. Measurements were also made as late or early as possible in the day when penetration of the canopy by direct sunlight is minimised. Measured values of LAI for the barley and wheat canopies are plotted as a function of day of year (doy) in figure 3.10. Also shown are estimates of LAI derived from BPMS canopies generated from the manually measured canopy structural data. These values are presented explicitly in table 3.2.
Figure 3.10 Measured and modelled LAI for barley and wheat.

It can be seen that there is a wide spread of measured LAI values for some canopies during development, resulting in a relatively poor agreement between the measured and modelled values in some cases. The likeliest cause of this divergence is the intra-field variability of measured LAI: the coverage of the barley canopy of 13th May (ba_119) varied from 10% to 70% across the field.

Table 3.2 Values of LAI derived from BPMS canopies.

<table>
<thead>
<tr>
<th>canopy</th>
<th>LAI</th>
</tr>
</thead>
<tbody>
<tr>
<td>ba_112 18/04</td>
<td>0.70</td>
</tr>
<tr>
<td>ba_119 13/05</td>
<td>3.89</td>
</tr>
<tr>
<td>ba_119 04/06</td>
<td>3.16</td>
</tr>
<tr>
<td>ba_119 24/06</td>
<td>3.19</td>
</tr>
<tr>
<td>ww_23/03</td>
<td>0.09</td>
</tr>
<tr>
<td>ww_23/04</td>
<td>2.25</td>
</tr>
</tbody>
</table>
3.1.5 Airborne data

A variety of airborne data were collected by the NERC ARS aircraft over the Barton Bendish field site during the 1997 field campaign. Due to the weather, the dates on which data could be collected were not ideally spaced through the growing season (see below). In addition, atmospheric conditions were not ideal when airborne data could be obtained (clouds and/or haze). However, contemporaneous ground measurements of LAI and BRDF described above were made. The nature of the data collected by the NERC aircraft is as follows:

- **Daedalus 1268 Airborne Thematic Mapper (ATM) data** – radiometer measurements in 11 broadband channels in the visible/NIR, SWIR, and TIR. Parallel flight lines were flown over the scene to provide overlap which gives BRDF sampling in the central region of overlap due to the wide (70°) FOV of the sensor (Barnsley et al., 1997a). The data were recorded at an altitude of 3000m giving a spatial resolution of around 5m. Forty three flight lines were flown in total, on three dates: 5/6/97, 2/8/97 and 6/8/97, each of which was accompanied by contemporaneous ground measurements of the properties described above. An ATM image of the field site is shown in figure 3.11.

- **Compact Airborne Spectrographic Imager (CASI) data** - hyperspectral radiometer data, consisting of 288 channels in the visible/NIR, obtained concurrently with the ATM data. Forty two flight lines were flown in total, on the dates given above, with a spatial resolution of approximately 3 m.

- **Colour aerial photography** - obtained concurrently with the ATM and CASI data. The resolution of the photography is approximately 2m (see figure 3.1).
3.2 Summary of field measurements and validation

The fieldwork described above was designed to provide information permitting validation of simulations of $\rho_{\text{canopy}}$. In particular, measurements of structural and radiometric canopy properties were designed for comparison with modelled properties derived from a full 3D (BPMS) structural model of the canopy. A number of general difficulties of conducting such fieldwork were encountered, in addition to specific problems caused largely by the weather conditions of summer 1997, which was an unusually wet summer.

In general, the BPMS estimates of canopy structural parameters agreed relatively well with the measured parameters. Given the inter- and intra-field variability of the crops agreement between measured and modelled values of %cover and LAI were generally good. Agreement of the measured and modelled values of canopy were not always so good but this is largely a function of the changing atmospheric conditions and the
uncertainty of what is being viewed through the radiometer IFOV (to better characterise this variability, simulations should be performed using an equivalent size IFOV). Even a small wind can move the canopy enough to change this dramatically, particularly at low canopy LAI when soil can be very visible. Given these constraints, it was concluded that the BPMS characterisation of canopy structure was more than sufficient for the experimental work described in succeeding chapters.
4 Examination of volumetric and GO scattering behaviour

The basis of the linear kernel-driven BRDF models described in chapter 2 is the assumption that $\rho_{\text{canopy}}$ can be described by a sum of one or two representative BRDF ‘shapes’, each approximating the behaviour of a separate component of canopy reflectance. Studies have shown that certain (angular) features of canopy reflectance are common to many types of vegetation (Kimes, 1984; Walthall et al., 1985; Goel, 1988; Barnsley et al., 1997b). Such features include the hotspot, increasing reflectance with view zenith angle (bowl shape) and the asymmetry of the bowl-shape caused by increased reflectance in the backscatter direction. In practice these features are modelled using a weighted sum of isotropic, volumetric and GO scattering components, each of which is a function of viewing and illumination geometry only (Wanner et al., 1995). This was introduced in equation 2.27.

As described in section 2.5.4, the volumetric kernels are approximations to the solution of radiative transfer in a plane parallel homogenous medium (Ross, 1981; Wanner et al., 1995). The GO kernels are derived from considering the proportions of sunlit and shadowed ground and canopy components from the illumination of spheroids randomly distributed on a Lambertian surface (Li and Strahler, 1986, 1990, 1992; Wanner et al., 1995). In both cases a variety of approximations are made to the physically complete solutions to allow the kernels to be formulated as linear functions of viewing and illumination angles only. They can then be summed to describe the BRDF of arbitrary surfaces. Most importantly, they can be linearly scaled (spatially) and applied to heterogeneous surfaces at arbitrary resolution (ignoring adjacency effects), typically 100s of m to km-scale (Lucht et al., 1999).

Linear kernel-driven BRDF models have been practically applied to airborne, spaceborne and field-measured multi-angular reflectance data and have been shown to fit observed data well (Roujean et al., 1992; Privette and Vermote, 1995; Hobson et al., 1999; Lewis et al., 1999). In addition, such models have been inverted against reflectance data to produce model parameters estimates, which in turn have been used to derive integrated quantities such as surface albedo (Barnsley et al., 1997b; Disney et al., 1997; Lewis et al., 1999; Strugnell and Lucht, 1999; Schaaf et al., 1999). There is ample evidence to suggest that the linear models are sufficiently flexible to describe the shapes of a variety of directional reflectance features. More recently, linear kernel-driven BRDF
models are being used to produce the first global spatial albedo products from MODIS directional reflectance measurements have (Schaaf et al., 1999, 2000a,b).

Given the approximations underlying the kernels it is perhaps surprising that the linear models are able to represent the form of surface reflectance so well. The kernels are severe simplifications of the physical solutions for volumetric and GO scattering from anisotropic surfaces, which are approximations in themselves. Further simplifications are needed in both cases to make the kernels linear functions of \( \theta \) and \( \theta_v \) only. Considering these various degrees of approximation, two questions regarding the modelling of scattered radiation by the linear kernel-driven BRDF models can be asked:

- **How are kernel-driven models able to adequately describe complex scattering from such a wide variety of surfaces, given their approximate nature and the simplifications they contain?**

- **What biophysical information (if any) is contained within the linear model parameters, and is it possible to extract and exploit such information from model inversion against measured reflectance data?**

These two questions form the basis of the work presented in this thesis. Linear models have been designed for use in processing global moderate resolution data sets because of their simplicity, linear scaling and rapid inversion properties. The application of linear models to process global MODIS data means it is now vitally important to understand both the limits of operation of the kernel-driven models and the information that may be accessible through their inversion.

This chapter presents results of experiments exploring the validity of modelling BRDF as a linear combination of volumetric and GO components. Chapter 5 presents further analysis of the information contained in the model parameters, and explores to what extent the kernels act independently. In chapter 6 knowledge gained from these experiments is applied to the development of a new linear kernel-driven model of BRDF with a spectral component. Chapter 7 proposes how improved kernel-driven models of BRDF might be applied to air- and space-borne data.
4.1 Experimental method

In order to investigate how linear models are able to describe scattering from vegetation canopies, a method of examining the underlying scattering behaviour occurring within the canopy has been developed. Measured 3D plant parameter data (described in section 3.1.5) have been used within the BPMS to simulate the scattered radiation field of developing barley and winter wheat canopies. The BPMS permits scattered radiation to be analysed purely in terms of the controlling geometric factors such as the proportions of sunlit and shaded canopy and soil. Scattering behaviour can also be analysed independently of wavelength, which is essential if conclusions are to be drawn regarding the operation of the kernel-driven models: they are formulated purely as functions of viewing and illumination angle and not wavelength. Using the measured 3D plant data within the BPMS, an investigation of the scattering behaviour of the canopy under arbitrary viewing and illumination conditions can be carried out. Any assumptions made in the BRDF models under consideration can also be replicated, making it the ideal tool for benchmarking BRDF modelling techniques (Lewis, 1999).

The barley and wheat canopies were chosen because their properties differ sufficiently from those postulated in the formulation of the kernels so that they should provide a difficult test case for the linear models:

- They are row crops (azimuthal variability).
- They are not horizontally homogenous (clumping, and variable density).
- They do not have a uniform, spherical LAD.
- They do not exist over a Lambertian surface (non-Lambertian soil).

In addition to these factors, there are a number of other departures from the assumptions made in the linear models common to all canopies. Radiometric properties may differ from those assumed (e.g. $p_{\text{leaf}} \neq \tau_{\text{leaf}}$); shadows within the canopy are not perfectly black (diffuse illumination will always be present); illuminated crown and ground regions are not likely to be equally bright. These canopies will provide a sterner test of the kernels’ ability to describe BRDF than canopies which closely conform to the assumptions of the models. If the models can adequately describe the BRDF of the chosen canopy, then they are likely to work in less demanding cases, where less of the assumptions made in the linear models are violated. Information regarding (non canopy-
specific) scattering behaviour derived from these canopies will be generally applicable. A secondary reason for selecting these crops is that agricultural canopies are of commercial and scientific interest to end-users attempting to derive biophysical parameter information from moderate resolution EO data (Lucht and Roujean, 2000).

Canopy reflectance generated using the ray tracing component of the BPMS software provides a full numerical solution for scattering within a simulated canopy (referred to subsequently as BPMS, or BPMS-generated) (Lewis, 1999). It is used here as a ‘baseline case’ i.e. it is assumed to be the single scattered bidirectional reflectance of the measured canopy under given viewing and illumination conditions, with the specified reflectance and transmittance behaviour of the canopy components. Results in chapter 3 support this assumption, demonstrating that the BPMS simulations using measured plant data are capable of accurately representing the observed features of the field-measured canopy reflectance, at the correct (angular) magnitudes. Derived structural parameters such as LAI, % cover and joint gap probability also agree within experimental limits (given the variability of measured values), although there is significant variability.

Recalling section 2.5.4, the assumption underpinning the linear kernel-driven BRDF models is that canopy reflectance may in general be considered as a linear superposition of volumetric and GO scattering components (Roujean et al., 1992; Wanner et al., 1995). The assumptions are made that \( \rho_{i} = k \tau_{i} \) for canopy elements (\( k \) is constant, unity in this case), and that only single scattering interactions are considered. It follows that canopy reflectance, \( \rho_{\text{canopy}} \), can be expressed simply as a linear sum of the scattering from the canopy and soil respectively i.e.

\[
\rho_{\text{canopy}} = \rho_{\text{leaf}} \alpha + \rho_{\text{soil}} \beta
\]

If equation 4.1 is compared with equation 2.27 (ignoring the isotropic term for the present) then, as a result of the single scattering assumption (i.e. soil→leaf and leaf→soil scattering events are precluded) the \( \rho_{\text{leaf}} \alpha \) term must represent the volume scattering component of \( \rho_{\text{canopy}} \), and the \( \rho_{\text{soil}} \beta \) term must represent the GO component. The volume scattering component, \( \alpha \), **must originate purely from the vegetation elements within the canopy** (and is therefore related to LAI) as there can be no leaf→soil interaction; similarly, the GO component must originate purely from the soil. If this is the case, then \( \beta \)
is simply the proportion of sunlit soil visible to the viewer, and is hence a function of \( \theta_i \) and \( \theta_v \) (as well as the inherent LAI and LAD of the canopy). These two components of \( \rho_{\text{canopy}} \) are illustrated in figure 4.1 which shows two nadir simulated images of a barley canopy in early stages of growth. In the left image \( \rho_{\text{leaf}} = 1, \tau_{\text{leaf}} = 0 \) and \( \rho_{\text{soil}} = 0 \) i.e. white areas correspond to sunlit vegetation and black areas to sunlit soil. In the right image \( \rho_{\text{leaf}} = 0 \) and \( \rho_{\text{soil}} = 1 \) i.e. black areas correspond to vegetation and white to soil.

**Figure 4.1** Components of \( \rho_{\text{canopy}} \): left image \( \rho_{\text{leaf}} = 1, \tau_{\text{leaf}} = \rho_{\text{soil}} = 0 \) (volume scattering); right image \( \rho_{\text{leaf}} = \tau_{\text{leaf}} = 0, \rho_{\text{soil}} = 1 \) (GO scattering).

Recalling the form of the volume scattering kernels (2.5.4.1.1) the volume scattering component of canopy reflectance is given as (c.f. equation 2.23):

\[
\alpha = \frac{P(\theta_i, \theta_v, \Phi)}{4G \mu \mu'} \left\{ 1 - e^{-\text{LAI} \left( \frac{G' G}{\mu \mu'} \right)} \right\}
\]

\( P(\theta_i, \theta_v, \Phi) \) is the single scattering phase function, LAI is the leaf area index, \( G' \) and \( G \) are the leaf projection functions in the viewing and illumination directions, and \( \mu \) and \( \mu' \) are the cosines of \( \theta_i \) and \( \theta_v \) respectively. Note that both \( \alpha \) and \( \beta \) are functions purely of viewing and illumination angle (and row azimuth in the case of row crops). As a result, any investigation of these parameters will be independent of wavelength. This is highly desirable for examining the operation of the linear kernel-driven (angular) models due to their reliance on purely geometric terms. Any conclusions that can be drawn will be solely concerned with geometric dependencies and not spectral ones.
4.2 Exploring the hypotheses behind the linear models

The linear kernel-driven approach to modelling BRDF is based on two fundamental and linked hypotheses, the first of which shall be examined in detail in the subsequent sections of this chapter, and the second in chapter 5:

1. Canopy reflectance can be modelled as a linear combination of volumetric and GO scattering components.

2. The volumetric component of $\rho_{\text{canopy}}$ is adequately modelled by the volume scattering kernel alone and similarly, the GO component is adequately modelled by the GO kernel.

All other properties of the linear models are reliant on the validity of these two hypotheses. If either proves unreliable then it can be concluded that the linear kernel-driven approach to modelling $\rho_{\text{canopy}}$ may need to be reconsidered. By testing them it is possible to demonstrate whether (and how) the linear models are capable of modelling a variety of different canopy types and surfaces. In addition it is hoped that the limits of their operation can be explored and extended. As noted previously, the kernels are designed to operate on heterogeneous surfaces at moderate resolution. In order to explore the scattering processes within canopies in detail however, we consider homogeneous surfaces at high resolution (cm).

4.2.1 $\rho_{\text{canopy}}$ as a linear combination of volumetric and GO scattering

The initial part of this experiment is designed to test hypothesis 1 above – namely that $\rho_{\text{canopy}}$ can be satisfactorily modelled as a linear combination of volumetric and GO scattered components. That is, can the two components be linearly related to the (purely geometric) terms governing the scattering from the vegetation and soil i.e. $\alpha$ and $\beta$ in equation 4.1? If the assumption of linearity is valid, it is vital to know under what conditions this assumption will hold and where it is likely to break down.

In order to test the hypothesis, BRFs were generated using measured plant parameter data characterising the 3D structure of barley (four dates) and winter wheat
(two dates). The structural data measurements described in detail in chapter 3. Values of LAI and % cover are given for the various canopies in table 4.1 and simulated views of each canopy are shown in figures 4.2a-f.

Table 4.1 Details of the canopies used in simulations

<table>
<thead>
<tr>
<th>Canopy</th>
<th>Date</th>
<th>LAI</th>
<th>% cover</th>
</tr>
</thead>
<tbody>
<tr>
<td>barley</td>
<td>18th April</td>
<td>0.56</td>
<td>15.1</td>
</tr>
<tr>
<td>barley</td>
<td>13th May</td>
<td>3.44</td>
<td>66.3</td>
</tr>
<tr>
<td>barley</td>
<td>4th June</td>
<td>3.14</td>
<td>62.9</td>
</tr>
<tr>
<td>barley</td>
<td>24th June</td>
<td>3.15</td>
<td>66.9</td>
</tr>
<tr>
<td>winter wheat</td>
<td>23rd March</td>
<td>0.08</td>
<td>3.4</td>
</tr>
<tr>
<td>winter wheat</td>
<td>23rd April</td>
<td>2.03</td>
<td>25.8</td>
</tr>
</tbody>
</table>

The simulated canopies shown in figure 4.2 are (arbitrarily) pictured as 1m² patches. Much larger areas are used for subsequent experimentation, with only small central sub-regions of each canopy being viewed in order to avoid 'edge effects' (see below). Such errors are caused by the divergence of the canopy from the assumption of infinite horizontal extent. During simulation, rays escaping the scene from beyond the horizontal extent of the canopy will lead to inconsistencies in the integration of exitant scene radiation. Additionally, if the modelled canopy is the same area as the area being viewed, some plant organs may extend beyond the edge of the scene leading to the possibility that there may be non-integer numbers of plants in a given area. It should be noted that the canopies in figure 4.3 are simulated over a non-Lambertian soil surface based on observed soil properties. The soil brightness characteristics have been modelled on the observed semivariance of soil properties extracted from photographs from the respective canopies. The height variation of the soil (due to the ploughing and drilling) is modelled using a sine function with the wavelength and amplitude determined from observed soil roughness characteristics. Small amplitude Gaussian noise has been added to the sine function to simulate small-scale surface roughness variations. In subsequent simulations used in this chapter and chapters 5 and 6, the soil is a simple Lambertian surface (as is assumed in the linear kernel-driven modelling approach).
Figure 4.2 Simulated images of measured barley and wheat canopies.
The viewed area of each canopy is designed to contain an integer number of rows (seven) resulting in a viewed area of 0.49m on a side (row spacing is 7 cm). The horizontal extent of the canopy, $l$, is chosen to be 0.49m plus twice the ground projection of the tallest part of the canopy (h) at an angle greater than the maximum $\theta_v$ to be used. In order to be safe, $\theta_v$ (max) of 70° is assumed even though in subsequent experiments $\theta_v$ never exceeds 60°. Therefore $l = 0.49 + 2htan\theta_v = 0.49 + 5.5h$. This ensures the modelled canopy extends sufficiently either side of the viewed area to eliminate edge effects, even at extreme $\theta_v$. For example, the barley canopy of 13th May has $h_{\text{max}} = 0.38m$ giving $l = 0.49 + 2(1.04)$ i.e. the canopy is extended to 1.04m on either side of the 0.49m central patch, giving a canopy of 2.57m on a side. Orthographic viewing projection is used to enforce parallel ray geometry. This ensures that the same area of surface is viewed regardless of $\theta_v$. As a result, the linear dimensions of off nadir scenes increase (relative to nadir) to ensure the same area is included in the simulation. This configuration is illustrated in figure 4.3.

![Figure 4.3 Viewing and illumination geometry and canopy extent for simulations.](image)
BRFs were simulated in the manner described above under the explicit assumptions of the linear models (see section 2.5.4) i.e.:

- single scattering interactions only
- bi-Lambertian leaf reflectance
- $\rho_{\text{leaf}} = \tau_{\text{leaf}}$ (values: 0.5 or 0)
- $\rho_{\text{soil}}$ is Lambertian (values: 0 or 1)
- direct illumination only

Directional reflectance was simulated in the solar principal plane at $\theta_v$ from $-60^\circ$ to $60^\circ$ in steps of $10^\circ$, except within the $10^\circ$ interval centred on the hotspot, where sampling was increased to every $2^\circ$. The row azimuth angle ($\phi_{\text{row}}$) of the crop was fixed at angles of $0^\circ$, $45^\circ$, and $90^\circ$ to the viewing plane, in order to provide the most extreme cases for analysis. This is likely to affect canopies with noticeable gaps between rows e.g. young crops. As $\phi_{\text{row}}$ increases shadowing will shift from along to across the rows. Figure 4.4 shows an example of simulated directional reflectance of the 13th May barley canopy ($\theta_v = \phi_{\text{row}} = 0^\circ$). The transition of dark to light with increasing view zenith is quite clear, including the bright hotspot image at nadir (differing aspect ratios are caused by the orthographic projection). Three wavebands are simulated: 450, 500 and 650nm, with corresponding $\rho_{\text{leaf}} = 0.062, 0.093$ and 0.068; $\tau_{\text{leaf}} = 0$; $\rho_{\text{soil}} = 0.123, 0.118$ and 0.132.

**Figure 4.4** Simulated barley reflectance, $\theta_v$ from $-50^\circ$ to $0^\circ$ (left to right, top to bottom).

If there is a linear relation between the volumetric and GO components of canopy reflectance and the volumetric and GO kernels, $k_{\text{vol}}$ and $k_{\text{GO}}$, then comparing equation 4.1 with the general linear model form of equation 2.27, $k_{\text{vol}}$ must be proportional to $\alpha$ and
$k_{GO}$ must be proportional to $\beta$. In this case, it can be said for BPMS-simulated canopy reflectance that (under these specific conditions):

\[
k_{vol} = a_{vol}\alpha + b_{vol}
\]

\[
k_{GO} = a_{GO}\beta + b_{GO}
\]

where $a_{vol}$, $b_{vol}$, $a_{GO}$, $b_{GO}$ are constants. Following equation 4.1 the simulated canopy reflectance can be divided into separate volumetric and GO scattering components (scattering from vegetation and soil only) to give values of $\alpha$ and $\beta$. If hypothesis 1 is valid then $\alpha$ and $k_{vol}$, and $\beta$ and $k_{GO}$ should be linearly related. Slopes of regressions of these parameters will yield $a_{vol}$ and $b_{vol}$, and the intercepts, $a_{GO}$, $b_{GO}$. The following section presents results of the BPMS simulations $\rho_{canopy}$. Results are also presented from regressing the volume and GO scattering components of the BPMS-simulated $\rho_{canopy}$ ($\alpha$ and $\beta$) against the values of $k_{vol}$ and $k_{GO}$ for the same viewing and illumination conditions.

**4.2.2 Volumetric and GO components of $\rho_{canopy}$**

The shapes of the volume and GO scattering components of $\rho_{canopy}$ for the barley and wheat canopies are presented here and discussed in section 4.2.3. Results of the regressions of $\alpha$ and $\beta$ against $k_{vol}$ and $k_{GO}$, along with discussion of these results, are presented in section 4.3.

Figure 4.5 shows the variation of the BPMS-derived volumetric parameter, or leaf-scattered component of simulated reflectance ($\alpha$ from equation 4.2) as a function of view zenith angle for four dates throughout the development of the barley (4.5 a-d) and wheat crops (4.5 e-f). Results are shown for $\theta_v$ ($0^\circ$, $30^\circ$, $60^\circ$) and for $\phi_{row}$ ($0^\circ$, $45^\circ$, $90^\circ$). Figure 4.6 a-f shows the variation of the BPMS-derived GO parameter of the various canopies ($\beta$ from equation 4.1), the soil-scattered component, under the same viewing and illumination conditions (NB note the changes of scale that occur between each of the figures a-f).
Figure 4.5 Variation with view zenith angle of BPMS-derived volumetric component of barley and wheat canopy reflectance for six dates.

a) barley – 18th April

b) barley – 13th May
c) barley - 4\textsuperscript{th} June

d) barley - 24\textsuperscript{th} June
c) wheat – 23rd March

f) wheat - 23rd April
Figure 4.6 Variation with view zenith angle of BPMS-derived GO component of barley and wheat canopy reflectance for six dates.

a) barley – 18\textsuperscript{th} April

b) barley – 13\textsuperscript{th} May
c) barley – 4\textsuperscript{th} June

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure_c.png}
\caption{Graph showing BPMIS GO parameter for different view zenith angles.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure_d.png}
\caption{Graph showing BPMIS Vol. parameter for different view zenith angles.}
\end{figure}

d) barley – 24\textsuperscript{th} June
e) wheat – 23rd March

f) wheat – 23rd April
4.2.3 Discussion of directional shapes and magnitudes of $\alpha$ and $\beta$

4.2.3.1 Volumetric component of $\rho_{\text{canopy}}$, $\alpha$

Figure 4.5 shows the volumetric component of BPMS-simulated $\rho_{\text{canopy}}$ to have (in general) an asymmetric, upward bowl-shape in the case of the barley canopy ($\alpha_{\text{barley}}$). Reflectance tends to be low (minimum) at nadir or in the forward scattering direction, and increases in the backscatter direction (increasing $\theta_i$) with a sharp peak in the hotspot direction. $\alpha_{\text{wheat}}$ is much flatter in comparison, showing a downward bowl-shape for all $\theta_i$, again with a sharp hotspot peak. $\alpha_{\text{wheat}}$ decreases between the 23$^{\text{rd}}$ March and 23$^{\text{rd}}$ April and the shape changes from a peaked downward bowl shape for $\theta_i = 0^\circ$ to a flat, almost upward bowl shape for $\theta_i = 60^\circ$. Variation with row azimuth ($\phi_{\text{row}}$) is negligible in both cases because the row and plant spacing are almost interchangeable (7cm and 5cm respectively).

Differences in the amount of vegetation account for differences in shape between $\alpha_{\text{barley}}$ and $\alpha_{\text{wheat}}$. In the wheat canopy of 23$^{\text{rd}}$ March there is virtually no vegetation present (LAI = 0.08, see figure 4.2e) and hence little vegetation scattering. In this case $\rho_{\text{canopy}}$ is simply determined by the amount of sunlit soil. The barley canopy of 18$^{\text{th}}$ April by contrast, has significant vegetation. Plots of the proportional contribution of the sunlit canopy components to scene reflectance for each canopy, shown in figure 4.7, support this. In each case, the fractional contribution of each scene component for each $\rho_{\text{canopy}}$ simulation (sunlit leaf, sunlit soil) is plotted with varying view zenith angle. Shadowed canopy components are not shown as they do not contribute to scene reflectance (no diffuse component of illumination, $\therefore$ shadows are perfectly black). $\rho_{\text{canopy}}$ will in this case be a combination of sunlit leaf and soil only, so the proportion$_{\text{sunlit leaf}} = 1 - \text{proportion}_{\text{sunlit soil}}$ (and vice versa). For comparison, the scene contributions from simulations of the same canopies but including diffuse illumination (i.e. shadowed components are non-zero) are given in Appendix 2. Recall that in each case, two 'synthetic' wavebands are simulated, the first in which $\rho_{\text{leaf}} = \tau_{\text{leaf}} = 0.5$ and $\rho_{\text{soil}} = 0$ i.e. in this case all signal is (by definition) single scattering from vegetation only; the second waveband has $\rho_{\text{leaf}} = \tau_{\text{leaf}} = 0$ and $\rho_{\text{soil}} = 1$ i.e. in this case all signal is (by definition) single scattering from soil only. Sunlit soil is the dominant scene component in both low LAI cases (figure 4.7a and e) and the behaviour of $\alpha$ reflects this. For wheat, sunlit soil represents greater than 85% of the total reflectance at all $\theta_{\nu,i}$. As the canopy develops, sunlit soil becomes prevalent.
Figure 4.7 Proportional contribution of sunlit scene components to total scene reflectance, for barley (four dates) and wheat (two dates).

a) barley – 18th April

b) barley – 13th May
c) barley – 4\textsuperscript{th} June

d) barley – 24\textsuperscript{th} June
(a) wheat - 23\textsuperscript{rd} April

(proportional contribution)

(b) wheat - 23\textsuperscript{rd} March

(proportional contribution)
A further difference between the crops which affects $\alpha$ is that in the early stages of growth the wheat canopy is quite strongly erectophile, which can cause dramatic variations in observed reflectance behaviour depending on $\theta_1$ and $\theta_2$ (Kimes, 1984; Goel, 1992). In an erectophile canopy, the LAD is biased towards higher leaf inclination angles (towards the vertical) so that visible vegetation is at a minimum closer to $\theta_1 = 0^\circ$ and increases relatively rapidly with $\theta_2$, while for the visible soil component, the converse applies. The cumulative LADs of the various canopies are shown in figure 4.8.

Figure 4.8 shows that the canopies all depart significantly from the assumption of a spherical LAD made in the formulation of the Ross kernels (section 2.5.4.1.1). The canopies generally tend towards an erectophile LAD i.e. the cumulative frequency distributions rise more slowly than the spherical case to begin with, then much more sharply at higher angles as more leaves are found with relatively high inclination angle. This is true to a greater or lesser extent for all canopies, but particularly wheat. Following the initial growth stages the wheat canopy becomes much more strongly erectophile than the barley. Although the modal LAD for both these canopies lies in the 85-90° range, the increase in frequency from the penultimate 80-85° range is 50% for wheat, and only 14%
for barley. Additionally, the mean LAD of the wheat canopy is 79.3° and 66.5° for the barley. The barley canopy of 24th June is closer to the spherical distribution than the others and also has far more leaves with lower inclination angles than any of the other distributions. However the structure of this canopy is strongly influenced by the seed heads, which cause the stems to 'bend down' under gravity (this can be seen in the photographs of figure 3.8). This canopy is also the most prone to permanent bending by prevailing winds - as a result of the seed heads again.

It is worthwhile to compare the canopy LADs with a theoretical distribution used in models of $\rho_{\text{canopy}}$ such as that of Bunnik (1978). Bunnik's approximation to LAD is a geometrical function with four parameters which can be varied to produce a range of desired distributions. Figure 4.9 shows the variation of Bunnik's theoretical LAD for five cases, erectophile (predominantly upright), extremophile (predominantly either erect or flat), plagiophile (predominantly mid-range), planophile (predominantly flat), spherical (all angles equally likely). Clearly, the barley and wheat canopies used here are closer to the erectophile LAD than any other. This is demonstrated in the correlation of measured canopy LAD values with Bunnik's LAD functions shown in figure 4.10. All canopies are relatively highly correlated with the erectophile distribution, except the 23rd April wheat canopy which has the lowest correlation with all LADs. The 24th June barley canopy does not follow the trends of the other canopies being nearly equally correlated with the erectophile, plagiophile and spherical distributions. This is a function of the change in canopy structure as it begins to senesce. Clearly, none of the canopies is planophile. The departure of the various canopies from the assumptions of a spherical LAD will tend to cause the scattering components of reflectance $\alpha$ and $\beta$, to depart from agreement with their respective kernels and $k_{\text{vol}}$ and $k_{\text{GO}}$. This is also likely to have consequences for the separability of scattering components.
Figure 4.9 Examples of Bunnik's LAD function.

Figure 4.10 Correlation of measured LAD against Bunnik distributions.
It is also instructive to examine the leaf projection functions $G(\Omega)$ (equation 2.21) and phase functions of the various barley and wheat canopies. Recall that $G(\Omega)$ describes the total fraction of leaf area (per unit volume of canopy) projected into the viewing direction, $\Omega$. Figure 4.11 shows $G(\Omega)$ for the various canopies for which the LAD are given in figure 4.8. $G(\Omega)$ is shown for $-90^\circ \leq \Omega \leq 90^\circ$.

Figure 4.11 Leaf projection function $G(\Omega)$ in viewing direction $\Omega(\theta_v, \phi_v)$.

Figure 4.11 shows the departure from the spherical LAD assumption of the various canopies, particularly the wheat canopy of 23\textsuperscript{rd} April. The closest to the spherical LAD is the barley canopy of 18\textsuperscript{th} April, for which $G(\Omega)$ varies from just below to just above 0.5. The largest departure is seen in the wheat canopy of 23\textsuperscript{rd} April, which has $G(\Omega)$ varying from 0.55 at $\theta_v = \pm 90^\circ$, down to 0.2 at nadir. This highlights the more erectophile nature of the canopy. Phase function is more directly a measure of canopy structure, describing as it does the angular distribution of scattering from the illumination direction $\Omega'$ into the viewing direction, $\Omega$, at each photon interaction. Figure 4.12 shows the variation of the phase function with view angle for the six barley and wheat canopies, for nadir illumination. Phase function varies with view angle with the wheat canopy of
23rd April having the lowest values and the barley canopy of 24th June having the highest values (and being most variable).

![Phase function graph](image)

**Figure 4.12** Phase function, for $\theta_i = 0^\circ$.

Returning to the various canopy scattering components, for the barley canopies of 18th April and 13th May (figures 4.5a and b), $\alpha_{\text{barley}}$ increases by a factor of four as $\theta_i$ increases from $0^\circ$ to $60^\circ$ at the forward scattering extreme ($\theta_r = 60^\circ$) where the variation is greatest. This increase of $\alpha_{\text{barley}}$ with increasing $\theta_r$ is even more pronounced in the developed canopies of figures 4.5c and d, with $\alpha_{\text{barley}}$ increasing by a factor of between 8 and 10 at $\theta_r = 60^\circ$. This behaviour is caused by more vegetation being visible at extreme angles, as seen in figures 4.7b to f. Proportions of sunlit leaf increase with $\theta_r$, with a corresponding reduction in sunlit soil. The shadowed leaf component also increases with $\theta_r$ but does not contribute in any way to scene reflectance. The magnitudes of $\alpha_{\text{wheat}}$ are similar to $\alpha_{\text{barley}}$ for canopies most closely corresponding in terms of LAI (18th April and 13th May). However the variation in magnitude of $\alpha_{\text{wheat}}$ with $\theta_r$ in the 23rd March case is much smaller than for barley. Values of $\alpha_{\text{wheat}}$ lie between 11 and 13 for all $\theta_i$, $\theta_r$, $\phi_{row}$. $\alpha_{\text{barley}}$ ranges between 0 and 8 and shows large variation with $\theta_s$, $\theta_r$, whilst for the 23rd April case, $\alpha_{\text{wheat}}$ varies between 0 and 12 depending on $\theta_i$, $\theta_r$. The contrast in behaviour
of $\alpha_{\text{wheat}}$ between the 23rd March (where the LAD resembles that of the 18th April barley canopy) to the 23rd April is again likely to be due to the increasingly erectophile LAD.

A feature of $\alpha_{\text{barley}}$ in particular (and $\alpha_{\text{wheat}}$ to some extent) is the asymmetry about $\theta_v = 0^\circ$ and the variation with $\theta_i$. This is easily explained by considering the proportions of sunlit leaf in figure 4.7. By definition, $\alpha$ represents the component of $\rho_{\text{canopy}}$ originating from sunlit vegetation. The proportions of sunlit leaf in figure 4.7 are increasingly asymmetric about $\theta_v = 0^\circ$, rising rapidly in the backscatter direction. This explains the behaviour of $\alpha$. In addition, varying $\theta_i$ will cause very different amounts of vegetation to be visible, leading to the variations in $\alpha$ with $\theta_i$.

The trends in magnitude of $\alpha_{\text{barley}}$ and $\alpha_{\text{wheat}}$ indicate that $\alpha$ is directly related to scattering from vegetation. Figure 4.5a shows $\alpha_{\text{barley}}$ varying from just above zero at nadir to almost 8 at $\theta_v = 60^\circ$ for the 18th April. $\alpha_{\text{barley}}$ rises to between 2-20 for 13th May, 3-28 for 4th June and then falls sharply back to below 2 for the 24th June at which point the barley has senesced prior to harvest. From this evidence it is clear that $\alpha$ is related to the quantity of vegetation present in the simulated canopies. The March 23rd (wheat) and April 18th (barley) canopies are characterised as a sparse arrangement of small plants with few tillers and leaves (figures 4.2a and e). Both crops rapidly develop into tall, densely packed canopies with almost complete coverage. The latter stages much more closely approximate the canopy envisioned in the formulation of the volumetric kernels, and reflectance from such a canopy can reasonably be expected to be dominated by the volumetric component. In addition, it is clear from equation 4.2 that the maximum in $\alpha$ will be when the $e^{-\text{LAI}}$ term approaches zero i.e. when LAI becomes large, in which case $\alpha$ tends to

$$\alpha = \frac{P(\theta_i, \theta_v, \phi)}{4G \mu \mu}$$

4.5

A clear feature of the variation of $\alpha$ in figure 4.5 is the increasing prominence of the peak in the backscatter direction at the point where the viewing and solar zenith angles are equal i.e. in the hotspot direction. This peak, caused by a maximum in the amount of visible sunlit scene components (and a corresponding minimum of visible shadow), is barely apparent in figure 4.5a as the canopy is very sparse. There is a lot of visible sunlit soil and very little shadowing, even at widely differing view and solar zenith angles. As can be seen in figure 4.7 (a and e) the scene reflectance of the 18th April barley
and the 23rd March wheat canopies are dominated by the amount of sunlit soil present, with shadowed soil and sunlit leaf having similar, much lower proportions. In the extremely sparse wheat canopy of 23rd March the sunlit soil component has a maximum of 0.95 and never falls below 0.8, meaning that the remaining components (sunlit or shadowed) are virtually negligible.

4.2.3.2 GO Component of ρ_canopy, β

The behaviour of the GO component of BPMS-simulated reflectance (β) shown in figures 4.6a-f contrasts with that of α. β_barley is initially an inverted bowl-shape (18th April, figure 4.6a), with a maximum at nadir and decreasing away from this point with increasing θ_v, but becomes slightly peaked at nadir as the canopy develops. β_barley has a maximum of approximately 0.8 at nadir viewing in the 18th April canopy and a minimum of 0.6 at θ_v = 60°. The nadir maximum falls to 0.35 by the 13th May, and falls further to between 0.1 and 0.2 in the most developed canopies of 4th and 24th June. For the 23rd March, β_wheat varies from 0.97 at nadir to 0.9 at θ_v = 60° and for the 23rd April β_wheat falls almost linearly from 0.8 at nadir to 0.05 at θ_v = 60°. β_wheat displays similar trends to β_barley, with close agreement in shape between β_wheat of 23rd March and β_barley 18th April, and β_wheat of 23rd April and β_barley 13th May. β_wheat has a larger range of variation in each case. The β_wheat and β_barley values of these dates are in much closer agreement than the corresponding α_barley and α_wheat. These trends (particularly the general downward bowl) are to be expected given that β is the proportion of sunlit soil visible to the viewer. From figure 4.6 it can be seen that in all cases the amount of sunlit soil reduces with increasing θ_v almost symmetrically about θ_v = 0° as more sunlit vegetation and shadowed soil/vegetation becomes visible. The exception to this is around the hotspot where shadowing is at a minimum. The magnitude of β in all cases is also directly comparable to the proportions of sunlit soil in figure 4.7. An unexpected result is the absence of a strongly peaked hotspot feature in β, as might be expected. However, this feature is clearly seen in the behaviour of the volumetric component α (where it is not expected), suggesting that α contains elements of behaviour that would only be expected for β. Possible reasons for this behaviour are posited below.
The transition in $\beta_{\text{wheat}}$ from the smooth downward bowl of 23rd March to the more sharply peaked case of 23rd April (seen to an extent in the barley canopy of 13th May) is explained by the much more erectophile LAD of the wheat canopy (particularly for the 23rd April canopy). In this case sunlit soil will tend to be at a maximum at nadir, dropping off sharply with increasing $\theta_v$ as the predominantly vertical leaves obscure the soil from view. In contrast, the barley canopy shows a more gradual reduction of sunlit soil with increasing $\theta_v$ away from nadir as a result of the less erectophile LAD.

The variations in magnitude of $\alpha$ and $\beta$ (particularly those of $\alpha$) support hypothesis 1 above (section 4.2), namely that $\rho_{\text{canopy}}$ can be separated into volumetric and GO components. If this is the case, $\alpha$ would be expected to be low in comparison to $\beta$ when the canopy is sparse, with $\rho_{\text{canopy}}$ dominated by the GO component of reflectance. In addition $\alpha$ might be expected to increase as the canopy develops to more closely resemble the plane parallel homogeneous medium approximated by the volumetric kernels, with a corresponding reduction in the GO component, $\beta$. This is precisely the trend observed. Results also show that there is a continuum of volumetric and GO scattering at all stages of growth. GO scattering is prominent at early growth stages when relatively large areas of sunlit soil are visible, with volumetric scattering taking over as the canopy coverage increases from sparse to dense. The fact that there appears to be elements of both volumetric and GO scattering implies that although it may be reasonable to assume two independent components of $\rho_{\text{canopy}}$, they are never likely to be perfectly separable. In particular, the behaviour of $\beta$ (lack of a hotspot) suggests that the canopies used here depart significantly from the assumptions made in the formulation of the GO kernels. In particular, the assumption of independent scattering crown "envelopes" is not valid.

It is important to note that the semi-empirical kernels were originally formulated based on the idea that the reflectance of heterogeneous scenes observed at moderate resolution could be characterised by proportions of scattering dominated by volumetric and GO scattering respectively (Wanner et al., 1997). These separate scattering components are considered to originate from separate patches within the scene, each contributing to the overall scene reflectance. $\rho_{\text{canopy}}$ considered at high resolution will have volumetric and GO scattering components present, although not quite as envisaged above. In the experiments presented in this thesis, the scattering from the canopy is being considered as a sum of volumetric and GO scattering components originating from within the same area of canopy. If the kernels cannot describe this case, then problems will arise.
at lower resolution simply because vegetation canopies are not typically homogeneous. At these scales there will be volumetric and GO components of $\rho_{\text{canopy}}$ originating from within the IFOV of a given sensor.

### 4.3 Conclusion

Values of $\rho_{\text{canopy}}$ for barley and wheat canopies at various stages of growth were simulated from measured canopy structural properties and field-measured soil and vegetation reflectance data. Simulations were carried out over a wide range of viewing and illumination configurations, under the assumptions made in the linear kernel-driven BRDF models ($\rho_{\text{leaf}} = \tau_{\text{leaf}}$, Lambertian soil, direct illumination and single scattering only). Volumetric and GO components of simulated $\rho_{\text{canopy}}$ were examined to see whether they can be treated as separate components as postulated in the formulation of linear, kernel-driven BRDF models. The trends in the magnitude of the volumetric and GO components of $\rho_{\text{canopy}}$ were as expected (other than the lack of a hotspot in the $\beta$ and the presence of one in $\alpha$):

- The volumetric component increased with LAI as the canopy developed, with the GO component reducing correspondingly.
- The variation of the volumetric component with $\theta_v$ was an asymmetric, upward bowl shape, with a peak in the hotspot direction and large variation with $\theta_v$.
- The GO component (dictated by the proportion of sunlit soil in this case) displayed a downward bowl-shape, symmetric about nadir, varying little with $\theta_v$, but without the expected hotspot.

The GO component of $\rho_{\text{canopy}}$ is related to the proportion of visible sunlit soil in each scene and the shapes and magnitudes of $\beta$ tend to support this. In contrast to $\alpha$, $\beta$ has a downward bowl-shape and is generally symmetric about nadir, with a maximum in the hotspot direction. It is important to note that the sharp hotspot peak that would be expected if $\beta$ were directly equated with sunlit and shaded soil components envisioned in the formulation of the GO kernels is not present. This is a result of the fact that $\rho_{\text{canopy}}$ was simulated using a canopy that departs very significantly from the assumptions made in the GO kernels described in section 2.5.4.1.2. In the formulation, the canopy is considered as

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a collection of 'spheroids-on-sticks' (see figure 2.10) and is modelled as a function of sunlit and shaded scene components. In the simulations presented above (and in subsequent analysis), shadows are perfectly black (no diffuse component of illumination) so the shadowed scene components contribute nothing to reflectance. In addition, the scattering objects in the scene are of a quite different shape and distribution from those shown in figure 2.10, with a much finer spatial scale and distribution within the canopy. These factors combine to prevent the appearance of the hotspot that would be expected if the canopy were composed of large, well-defined solid geometric objects envisaged in the formulation of the GO kernels. In fact, both the barley and wheat canopies resemble the configuration envisioned in the volumetric scattering kernels (see 2.5.4.1.1) far more closely than they do the GO scattering configuration (see 2.5.4.1.2). This would explain why the angular behaviour of $\beta$ is not quite as expected.

Differences between $\beta_{\text{barley}}$ and $\beta_{\text{wheat}}$ can be explained by differences in the LAD of the two canopies throughout their development: barley more closely approximates the spherical LAD assumed in the linear models; the measured wheat canopy has a more erectophile LAD, particularly for the 23rd April. The observed magnitude and behaviour of $\alpha$ and $\beta$ during the various stages of canopy development are strong evidence that $\rho_{\text{canopy}}$ can be split into volumetric and GO scattering components and that the information contained in each is largely independent of the other. However, results also show that even in canopies with very little vegetation there is a scattering component of reflectance that closely resembles the modelled volumetric component. Similarly, even canopies that have almost total coverage (i.e. virtually zero sunlit soil) a component of GO-like scattering remains. This indicates that although the two components may be generally separable in many cases, the extent to which this is true will depend closely on the nature of the canopy being studied. This implies the kernels need to be applied with care when the nature of the vegetation in the scene departs dramatically from that envisioned in the kernels (in particular mixed regions of clumped and well-distributed vegetation such as widely spaced trees with a grass understorey).

The next stage is to examine the relationship between the volumetric and GO scattering components of $\rho_{\text{canopy}}$ and the respective volumetric and GO scattering kernels, $k_{\text{vol}}$ and $k_{\text{GO}}$. The ability of the angular kernels to describe the respective scattering components is explored in chapter 5.
5 Canopy scattering and the linear model parameters

It has been established that the volumetric and GO scattering components of $\rho_{\text{canopy}}$ can largely be separated from each other on the basis of their angular behaviour. In addition, the respective scattering components can be related to the respective canopy elements from where they originate. The volumetric component, $\alpha$, is related to the proportion of sunlit vegetation visible to the viewer and hence the leaf scattering phase function. The GO component, $\beta$, can be related to the amount of sunlit soil visible to the viewer and hence reduces with increasing canopy coverage. It should be stressed that these findings relate to single scattering reflectance only. The linear kernel-driven models of BRDF assume single scattering interactions only and this is followed in the simulations of $\rho_{\text{canopy}}$ used here. The results discussion in this chapter examine the relationship between $\alpha$ and $k_{\text{vol}}$ and $\beta$ and $k_{\text{GO}}$.

5.1 Relationships between $\alpha$ and $k_{\text{vol}}$, and $\beta$ and $k_{\text{GO}}$

$\alpha$ has been defined to represent the volumetric scattering component of the BPMS-simulated $\rho_{\text{canopy}}$ (equation 4.2). It would therefore be expected that a linear relationship between $\alpha$ and $k_{\text{vol}}$, the volumetric kernels (equations 2.28 and 2.29) exists (when $f_{\text{vol}}$, the volumetric parameter, is inverted against reflectance data). $\beta$ is defined as the GO component of BPMS-simulated $\rho_{\text{canopy}}$ (equation 4.3) and it is similarly reasonable to expect a linear relation between the GO kernels, $k_{\text{GO}}$ (equations 2.30 and 2.31) and $\beta$. The first step in determining how accurately $k_{\text{vol}}$ and $k_{\text{GO}}$ describe $\alpha$ and $\beta$ is to plot the volumetric and GO kernels against the respective scattering components of $\rho_{\text{canopy}}$. As in chapter 4, values of $\rho_{\text{canopy}}$ simulated within the BPMS under the assumptions of the linear kernel-driven models of BRDF are employed.

Figure 5.1 shows plots of the BPMS-derived volumetric scattering component of $\rho_{\text{canopy}}$, $\alpha$, as the abscissa, against the RossThick and RossThin volumetric kernels for barley (four dates) and wheat (two dates). Figures 5.2 and 5.3 show the GO component of $\rho_{\text{canopy}}$, $\beta$, plotted against the LiSparse and LiDense kernels respectively. Plots are also

---

1 Both the reciprocal and non-reciprocal versions of the GO kernels were used in order to examine any differences in behaviour. Results for both were very similar, with the non-reciprocal version proving to be a marginally better fit in all cases. Consequently results from the non-reciprocal versions only are presented.
shown from two slightly modified versions of these kernels, which treat the reflectance of
the sunlit crown and sunlit ground independently, rather than assuming they are of equal
brightness as in the standard Li kernels (see figure 2.12). They are included to explore the
possibility that they might prove a better fit to the GO component of ρ_{canopy} than the
standard kernels. If so, they may provide a better interpretation of the GO component than
is the case in the original formulation of the models, given that sunlit and shaded crown
and ground are likely to be of different brightness in practice. The standard and modified
kernels are labelled G (for ground only) and GC (for ground and crown) respectively in
figures 5.2 and 5.3. Results are presented from simulated reflectance data from all solar
zenith angles and row azimuths combined, but the implications of treating individual
solar zenith and row azimuth angles separately are discussed below.

The view and illumination configurations considered in each case are as follows:

- ϕ_{row} = 0°, 45°, 90°;
- θ_τ = 0°, 30°, 60°;
- θ_σ in each case between -70° and 70°, in steps of 10° except for the 5° either side
  of the hotspot, where sampling is every 2°;

As described previously, single-scattering ρ_{canopy} is simulated in each case with two
nominal wavebands: one with ρ_{leaf} = τ_{leaf} = 0.5 and ρ_{soil} = 0; the other with ρ_{leaf} = τ_{leaf} = 0
and ρ_{soil} = 0. This results in scattering either from the vegetation (α) or from the soil (β).
These are plotted against their respective kernels in figures 5.1, 5.2 and 5.3. The lines in
each figure represent the regression line of each data set.
Figure 5.1 BPMS-derived volumetric component ($\alpha$) against $k_{\text{vol}}$ for barley (four dates) and wheat (two dates).

(a) barley – 18$^{\text{th}}$ April

(b) barley – 13$^{\text{th}}$ May
c) barley – 4$^{th}$ June

d) barley – 24$^{th}$ June
e) wheat – 23rd March

f) wheat – 23rd April
Figure 5.2 BPMS-derived GO component (β) against k_{GO} (LiDense) for barley (four dates) and wheat (two dates).

a) barley – 18th April

b) barley - 13th May
c) barley – 4\textsuperscript{th} June

d) barley – 24\textsuperscript{th} June
e) wheat – 23rd March

f) wheat – 23rd April
Figure 5.3 BPMS-derived GO component ($\beta$) against $k_{GO}$ (LiSparse) for barley (four dates) and wheat (two dates).

a) barley - 18th April

b) barley - 13th May
c) barley – 4\textsuperscript{th} June

d) barley – 24\textsuperscript{th} June
e) wheat – 23rd March

f) wheat – 23rd April
5.2 Variation of volumetric component, $\alpha$ with $k_{vol}$

5.2.1 Results

Figure 5.1 shows a generally linear relationship between the BPMS-derived volumetric scattering component $\alpha$ and the volumetric kernels, $k_{vol}$, particularly for the barley canopy. The relationship is less clear for wheat. Values of the correlation coefficient, $r$, are presented in tables 5.1. The value of $r$ is a direct measure of the sign of the correlation between two variables (positive or negative), but an indirect measure (square root) of the strength of the correlation. The coefficient of determination, $r^2$, represents the strength of correlation and is in effect the percent variance of the dependent variable explained by the regression equation. Clearly, $r^2$ can be calculated from values of $r$, but it is not possible to determine the sign of $r$ in this way, which is why only values of $r$ are given. Also included in table 5.1 are values of $a_{vol}$ and $b_{vol}$, the slopes and intercepts of the regression relationships. These results tend to support the first hypothesis presented in 4.2 that $\alpha$ is linearly related to the volumetric scattering kernels. An interesting feature of the results presented in table 5.1 is the variation in $r$ with the illumination (solar) zenith angle, $\theta$. While the variation with $\phi_{row}$ is minimal, $\theta$ appears to significantly affect the agreement between $k_{vol}$ and $\alpha$. Although we might expect $\alpha$ to be independent of $\theta$, an explanation for the variation is that the increased path length of radiation through the canopy from higher solar zenith angles sun will increase the volumetric scattering component of $\rho_{canopy}$ in relation to $\beta$. The values of $r$ increase, in some cases dramatically, with increasing $\theta$. The only cases where this is not clear are for the wheat canopies of March and April. In all cases for the barley canopies, the increases of $\alpha$ with $\theta$ are marked.

The RossThin kernel is included in this analysis to see whether evidence supports the adoption of the RossThick kernel for the MODIS albedo product (Lucht et al., 1999). The values of the RossThick and RossThin kernels in table 5.1 are separated by colour, with the RossThin values in red. All correlations presented in table 5.1 are significant to a 95% confidence level. Values in bold are those for which the upper and lower confidence levels lie within $\pm 0.125$ of the value of $r$, the correlation coefficient. This indicates correlations with the smallest confidence interval.

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Table 5.1 Slopes, intercepts and regression coefficients for volumetric kernels as a function of solar zenith ($\theta$) and row azimuth ($\phi_{row}$) (RossThin kernels in red).

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### 5.1d barley - 24th June

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### 5.1e wheat – 23rd March

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### 5.1f wheat – 23rd April

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5.2.2 Analysis of regression relationships

The results for $\alpha$ plotted against $k_{\text{vol}}$ presented in tables 5.1a-f, show $r$ starting high for the 18th April barley canopy, exceeding 0.96 in most cases, then falling slightly for the 13th May canopy to around 0.9. There is little difference between the RossThin and RossThick kernels for 18th April, but by the 13th May, the RossThick kernel has significantly higher values of $r$ than the RossThin at most $\theta_i$ and $\phi_{\text{row}}$. Values remain very similar for the June 4th barley canopy, but fall significantly for the 24th June. The RossThick kernel has significantly higher values of $r$ in this case, particularly for $\theta_i = 0^\circ$.

The results for the wheat canopy of 23rd March show little consistency, with values of $r$ between -0.93 (strong negative correlation) and 0.91, due to the fact that there is so little vegetation present. The values of $r$ for the RossThick kernel are always positive, and are relatively high (>0.8) for $\theta_i = 0^\circ$. The values for the RossThin kernel by contrast are predominantly negative. Although the RossThin kernel was formulated for describing the reflectance of sparse canopies (see 2.5.4.1.1), the vegetation in this case is so sparse as to be almost negligible. This may explain why the RossThin kernel does not correlate with $\alpha$ - there is little or no volumetric scattering. The RossThick kernel appears to fit well regardless, suggesting it is much more flexible than the RossThin in a variety of conditions, a finding supported by other researchers (Lucht et al., 1999; Strugnell and Lucht, 2000).

The results for the wheat canopy of 23rd April are similar to those of the barley canopy of 13th May and 4th June with the RossThick kernel providing a better fit in nearly all cases. For all $\phi_{\text{row}}$, $r$ values for the RossThick kernel are high for both $\theta_i = 0^\circ$ and $\theta_i = 60^\circ$, but are much lower for $\theta_i = 30^\circ$. Values of $r$ for the RossThin kernel display a clear trend: a strong negative correlation for $\theta_i = 0^\circ$, almost zero correlation at $\theta_i = 30^\circ$, and a relatively strong positive correlation for $\theta_i = 60^\circ$, again for all $\phi_{\text{row}}$. The RossThick kernel is far more stable in all cases.

As discussed in section 2.5.4.1, the Ross kernels are based on a solution of radiative transfer in a homogeneous (turbid) medium. The thick and thin versions of the Ross kernels result from approximations for LAI $\gg$ 1 and LAI $\ll$ 1 respectively. It might therefore be expected that the RossThin kernel would correlate with $\alpha$ more closely for the sparse canopies where LAI < 1 (i.e. the 18th April barley and 23rd March wheat canopies) and the RossThick kernel to correlate more strongly for the remaining canopies.
where LAI exceeds 2. This is marginally true for the 18th April barley canopy, but not at all the case for the 23rd April wheat canopy, where the RossThin kernel is often negatively correlated with $\alpha$. This is the sparsest canopy, with very little vegetation present and yet the RossThick kernel is more strongly correlated with $\alpha$, although only at a significant level for $\theta_i = 0^\circ$. This is a surprising result as the canopy departs not only from the assumption of high LAI, but also from the fundamental assumption of a turbid medium common to both kernels. This suggests that either the two components of $\rho_{\text{canopy}}$ cannot be simply separated, or that the $k_{\text{vol}}$ kernels not only explain variations in $\rho_{\text{canopy}}$ caused by volumetric scattering but also describe some aspects of GO scattering. For the more developed canopies the RossThick kernel is more closely correlated with $\alpha$, having consistently high (>0.85) values of $\gamma$. Results for the 23rd April wheat canopy are similar to those of the denser barley canopies. The exception is that values of $\gamma$ for the RossThick kernel fall significantly (to -0.5) for $\theta_i = 30^\circ$. This may be a result of the erectophile LAD mentioned previously (figure 4.8).

This behaviour is consistent with previous results: the volumetric component of $\rho_{\text{canopy}}$, $\alpha$, is strongly linearly related to $k_{\text{vol}}$ until the canopy rapidly senesces during the middle of June and there is little or no green vegetation remaining (e.g. although the barley LAI stays constant at around 3.15 in June, by 24th June, very little of the remaining vegetation is green). The RossThick kernel is favoured for nearly all dates except the 18th April barley canopy, despite variations in LAI. This is true even of the 23rd March wheat canopy with LAI = 0.08. The ability of the RossThick kernel to out-perform the RossThin kernel has been found by other researchers (Lucht et al., 1999; Strugnell and Lucht, 2000). This evidence supports the selection of the RossThick kernel as the volumetric kernel for production of global BRDF and albedo products from MODIS (Schaaf et al., 2000a, b).

5.2.3 Slopes and intercepts $a_{\text{vol}}$, $b_{\text{vol}}$ of $\alpha$ against $k_{\text{vol}}$

The slopes of $k_{\text{vol}}$ against $\alpha$ ($a_{\text{vol}}$) are small and generally positive (0 < $a_{\text{vol}}$ < 1). The intercepts ($b_{\text{vol}}$) are non-zero and almost exclusively negative. Following the convention of Roujean et al. (1992) that the volumetric kernels should equal zero for $\theta_i = \theta_r = 0^\circ$, the RossThick and RossThin kernels contain offsets of $-\pi/4$ and $-\pi/2$ (-0.79 and -1.57) respectively (equations 2.28 and 2.29). The values of the intercepts in table 5.1 are
close in magnitude to these values - further evidence that the volumetric component of $\rho_{\text{canopy}}$ can be separated from the GO component and represented by a relatively simple semi-empirical function. As detailed in section 2.5.4.1 the gradients correspond to the expressions $\frac{4 \rho_{\text{leaf}}}{3\pi} (1 - e^{-LAI})$ for the RossThick kernel, where B is a constant with a value of 1.5 (B is in fact a function of $\theta_i$ and $\theta_v$ but only varies between 1 and 2, so a value of 1.5 is chosen in order to simplify the kernels) and $\frac{2 \rho_{\text{leaf}} LAI}{3\pi}$ for the RossThin kernel.

Examining the values of $a_{vo/}$, $b_{vo/}$ and $r$ in table 5.1 according to solar zenith angle $\theta_i$ shows some interesting trends. In the 18$^{th}$ April case the RossThick kernel appears significantly better than the RossThin kernel except for $\theta_i = 0^{\circ}$, when $r$ is negative and $< 0.7$, implying a weak negative correlation. For the other dates the regression of the RossThin kernel produces negative values of $r$ where $\theta_i = 0^{\circ}$.

5.2.4 Summary

$k_{vo/}$ is generally strongly correlated with $\alpha$, the volumetric component of $\rho_{\text{canopy}}$, more so for dense canopies than sparse. There is very little variation in correlation with row azimuth angle, $\phi_{row}$, but considerable variation with illumination angle. For the barley canopy, correlation is low between the RossThick kernel and $\alpha$ for the sparse (18$^{th}$ April) canopy. This is particularly true at nadir illumination where little volumetric scattering is present. Correlation between RossThin kernel and $\alpha$ is much higher here. Correlation between RossThick and $\alpha$ increases as the canopy develops, as expected. Conversely, correlation with RossThin reduces and becomes much more strongly dependent on $\theta_i$. This is likely to be a result of increased volumetric scattering at high $\theta_i$ due to increased path length though the canopy. For senescent barley (24$^{th}$ June) the correlation between $\alpha$ and RossThick reduces rapidly with increasing $\theta_i$, and correlation with RossThin is generally low.

For wheat the correlation between the volumetric kernels and $\alpha$ is generally much lower than for barley. In addition, RossThick is more strongly correlated than RossThin for the sparse wheat canopy (23$^{rd}$ March), unlike the barley case. Correlation is also generally more variable with $\theta_i$. For the more developed wheat canopy (23$^{rd}$ April)
correlation between RossThick and $\alpha$ is much greater than for the sparse canopy. Correlation of RossThin increases from strongly negative to strongly positive with $\theta_i$. Observed differences between results for barley and wheat are likely to be due to structural arrangement of the canopy (e.g. LAD).

5.3 Variation of GO component, $\beta$, with $k_G$

5.3.1 Results

Results presented in figures 5.2 and 5.3 for the BPMS-derived GO component of $\rho_{\text{canopy}}$, $\beta$, against the LiDense and LiSparse kernels do not show such clear linear relationships as the plots of $\alpha$ against the volumetric kernels. There is a far greater spread of points than seen for the volumetric component, largely due to the variation between the separate $\theta_i$ cases. The correlation between the values of $\beta$ and the GO kernel values varies from being close to one in some cases, through zero to strong negative correlation in some cases. In addition, the differences of scale (an order of magnitude between ordinate and abscissa) result in low values of $r$. The slopes, intercepts and regression coefficients for $\beta$ against GO kernels are presented in tables 5.2 and 5.3. Table 5.2 contains the results from the LiDense and LiSparse kernels, while table 5.3 contains the results from the LiDenseGC and LiSparseGC variants. The kernels are labelled in the tables as follows:

- LiDense (G) $\Rightarrow$ DG
- LiDense (GC) $\Rightarrow$ DGC
- LiSparse (G) $\Rightarrow$ SG
- LiSparse (GC) $\Rightarrow$ SGC

As in table 5.1, the kernels are separated by colour, with the LiSparse (SG) values in table 5.2 and the LiSparseGC (SGC) values in table 5.3 being presented in red. Also as in table 5.1, all correlations are significant to a 95% confidence level. Values in bold are those for which the upper and lower confidence levels lie within $\pm0.125$ of $r$. This indicates correlations for which the confidence interval is smallest, suggesting a strong correlation.
Table 5.2 Slopes, intercepts and regression coefficients for the LiDense and LiSparse GO kernels as a function of solar zenith ($\theta_i$) and row azimuth ($\phi_{raw}$) (LiSparse kernels in red).

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150
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### 5.3f wheat – 23rd April

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5.3.2 Analysis of regression relationships

The results for $\beta$ against $k_{GO}$ presented in figures 5.2 and 5.3, and tables 5.2 and 5.3, show much greater variation than those seen for $\alpha$ against $k_{val}$, although some trends are similar. The variation of the correlation coefficient, $r$, with $\phi_{row}$ is negligible on the whole (as above) but there is significant variation with solar zenith angle, $\theta_z$ (also as above). Unlike the $\alpha$ case, it is expected for $\beta$ given that the GO component of $p_{canopy}$ will be strongly dependent on the amount of shadowing in the scene, which will vary with $\theta_z$ (and with the arrangement of objects within the canopy). The values of $r$ are generally high and positive at nadir illumination, reducing with increasing $\theta_z$, becoming predominantly negative. These trends hold for all kernels. The values of $r$ for the LiSparseGC (SGC) kernel, in the 18th April barley case (table 5.3a) reduce from 0.96 to -0.43 as $\theta_z$ increases from nadir to 60°. The exception to this trend is the barley canopy of 24th June where there is significant variation in $r$ with $\phi_{row}$. Although $r$ for $\phi_{row} = 0°$ follows the same trend as for the other canopies, the trend is reversed for $\phi_{row} = 45°$ and $\phi_{row} = 90°$ with $r$ starting low or negative for $\theta_z = 0°$ and increasing to the highest value at $\theta_z = 60°$. This is the only canopy with significantly different canopy structure, having mature seed heads, a somewhat different LAD (from figure 4.10, correlating much more

Figure 5.4 Perspective view of barley plants from above.
highly with the plagiophile, planophile and spherical LADs than any other canopy), and less green vegetation. Recent work has shown that the representation of these heads can significantly affect $\rho_{\text{canopy}}$, particularly single scattered radiation (Saich et al., 2001). Figure 5.4 is a perspective view of a barley canopy from above, with seed heads modelled as simple Lambertian cylinders. These cylinders contribute disproportionately strongly to $\rho_{\text{canopy}}$.

The standard LiSparse kernel performs significantly better in all cases than the standard LiDense kernel, with maximum values of $r$ almost always greater than 0.95 (although this is only true at $\theta_i = 0^\circ$) as opposed to values between 0.6 and 0.85 for the LiDense kernel (table 5.2a-f). In addition both the modified GC versions of the GO kernels perform better than the LiDense kernel, and perform comparably with the standard LiSparse kernel (table 5.3a-f). Correlations between $\beta$ and $k_{\text{GO}}$ for barley rise as the canopy develops before falling back for 24th June. The wheat canopies of 23rd March and 23rd April show much the same trends as for the barley. The results of the two barley and wheat canopies closest in terms of development (23rd March wheat, 18th April barley and 23rd April wheat, 13th May barley) show close agreement. This is in contrast to the results for correlations between $\alpha$ and $k_{\text{vol}}$.

The values of $r$ for the plots of $\beta$ against $k_{\text{GO}}$ suggest that is less clear that the GO component of $\rho_{\text{canopy}}$ is characterised by the linear function of $\beta$ proposed in equation 4.4 (unlike the situation for $\alpha$ seen in section 5.2). There is some agreement, but the variability of the results, particularly with varying $\theta_i$, suggests that the GO kernels do not work particularly well when faced with the row-based canopies comprised of relatively fine leaves used here. A consequence of this described in chapter 4 is the absence of a clear hotspot feature in the GO component of simulated $\rho_{\text{canopy}}$, $\beta$, and the presence of one in the volumetric component, $\alpha$. This departure from expectations is not altogether surprising given the departure of the barley and wheat canopies from the assumptions made in the formulation of the GO kernels i.e. spheroids randomly located on a Lambertian surface, with log-normal height distribution and perfectly black shadows. Figure 5.5 illustrates the type of canopy envisaged in the formulation of the kernels: a field of spheroids above a Lambertian surface. The heights are not log-normally distributed (as in the GO kernel formulation), but clearly it may not be realistic to expect the barley and wheat canopies shown in figures 4.2 to behave like the canopy in figure 5.5. One approach to the dependence on $\theta_i$ suggests that the GO kernels may need to be
more flexible in situations where the assumptions underlying the kernels are not met. In some cases, the GO kernels just may not be appropriate. A solution to the row dependent behaviour of the GO kernels might be to define a new set of GO kernels based on canopies with strong row orientations. This would allow a greater degree of confidence to be placed in the ability of the kernels to describe reflectance over agricultural regions.

Such kernels would not have random distributions of spheroids on sticks, but would have a dependency on row azimuth angle, $\phi_{row}$ (in relation to the viewer). In addition, taking account of the clumped vegetation that predominates when considering these high resolution scenes would improve matters, for instance by using effective LAI (LAI$_e$), rather than LAI directly for example (Nilson and Kuusk, 1989).

It has already been established that the GO component of $\rho_{canopy}$ as simulated in these experiments is determined by $\beta$, the proportion of sunlit soil (it should be noted that this differs from the theoretical case envisioned by Li and Strahler (1985, 1986, 1992) for example, which is driven by scene components including sunlit and shaded crown and ground. In this case, shadowed crown and ground contribute zero to scene reflectance (no diffuse illumination), so the GO component of $\rho_{canopy}$ by definition originates from the sunlit soil). Figure 4.6 shows that the proportion of sunlit soil is the dominant component of $\rho_{canopy}$ in the 18th April barley and 23rd March wheat canopies, accounting for the similarity in results of these two canopies. Although the proportion of sunlit soil varies in

![Figure 5.5 Simulated 'spheroids on sticks' canopy.](image)
the same way with $\theta_v$ for all canopies (downward bowl-shape, peak in the hotspot direction), the magnitude is very different, reducing from 0.6-0.8 (18th April, 23rd March) when the canopy is sparse, to close to zero for the 4th June (LAI = 3.19, 80-90% cover). The assumptions behind the GO kernels are more closely adhered to in the sparse canopies when the proportion of sunlit soil is highest and the regularly spaced plants with small leaf area are well-separated. Subsequent increases in cover reduce the proportion of sunlit soil, as well as the separability of the plants; they become a dense canopy rather than individual scattering objects. Consequently the GO component of $\rho_{\text{canopy}}$ is less-well characterised by equation 4.4. The decline in strength of the correlation with increasing $\theta_i$ suggests that the projected area of plants departs from the projections assumed in the GO kernels. Although the proportion of sunlit soil reduces with increasing $\theta_i$ it clearly does not do so in the manner assumed in theory (particularly in the case of the LiDense kernel). This is hardly surprising: the plants begin small, with leaves large in proportion to plant height; in the latter stages the plants are tall and very thin, with proportionally much smaller leaves. These plants are further removed from the spheroidal assumption than their immature counterparts. In addition, as the proportion of visible soil (sunlit or otherwise) reduces, the projected area of the plants will become proportionally more important.

5.3.3 Slopes and intercepts $a_{GO}$, $b_{GO}$ of $\beta$ against $k_{GO}$

In the same manner as seen in 5.2.3 for the volumetric kernels, the values of $a_{GO}$, $b_{GO}$ in tables 5.2a-f and 5.3a-f correspond to the slopes and intercepts of the regressions of $\beta$ against $k_{GO}$. The LiDense kernel contains an offset of −2 (equation 2.31) to ensure that the kernel is zero for nadir viewing and illumination (the LiSparse kernel is zero anyway under these conditions). The gradients are $CL\pi r^2$ for the LiSparse kernel, where $C$ is the reflectance of the sunlit crown (equal to 1), and $\lambda$ is the number density of spheroids on the surface of width $2r$, and $C/2$ for the LiDense kernel. Table 5.3a shows that in the 18th April case the values of $a_{GO}$ are mostly positive and vary from close to zero up to 14 or 15 for the LiDense (GC) kernel. Values of $b_{GO}$ are almost exclusively negative, varying from just below zero in most cases, down to −15 for the LiDense (GC) kernel. The values of $a_{GO}$ gradually increase for the barley canopy as it develops and the total scattering component increases, with the values of $b_{GO}$ remaining similar for each
date. The biggest changes are seen between the wheat canopies of 23rd March and 23rd April (tables 5.2 and 5.3 e and f). For the earlier canopy, the values of $a_{GO}$ and $b_{GO}$ are extreme, ranging from −25 to 65 in the case of $a_{GO}$, with $a_{GO}$ following similar patterns. However, for the 23rd April canopy the gradients and intercepts are comparable to the values in tables 5.2 and 5.3 a and b for the 18th April and 13th May canopies.

5.3.4 Summary

In most cases the correlation between $\beta$ and $k_{GO}$ (as measured by $r$, the correlation coefficient) is lower than that between $\alpha$ and $k_{vol}$. Results suggest that in certain cases the volumetric and GO scattering components can be separated and are generally linearly related to the respective kernels used to describe them in the linear kernel-driven models of BRDF, although there is significant variation in this relationship. For both barley and wheat there is little variation with $\phi_{row}$ in correlation in the earlier stages of the canopy. This changes for the 24th June barley canopy, when values of $r$ increase dramatically with increasing $\phi_{row}$. This is likely to be related to the structural variation in the canopy described above, with far less shadowed soil being visible as well as the presence of seed heads. There is significant variation in the strength of correlation with increasing $\theta_{i}$, with values of $r$ moving from high positive values at nadir to zero or negative values for $\theta_{i} = 60^\circ$. This trend is true for each barley canopy.

In the early stages of growth of both the barley and wheat canopies the sparse and dense variants of $k_{GO}$ are similar, with the sparse version having a slight edge in terms of correlation with $\beta$. The sparse variants become increasingly better as the canopy develops. This is further evidence to support the choice of the sparse family of kernels as the GO kernels-of-choice for BRDF and albedo production from MODIS reflectance data. The GC variants of $k_{GO}$, treating ground and crown as having separate reflectance, perform better in nearly all cases, in the sense of being more closely correlated with $\beta$. The only exception to this is in the 24th June barley case. In terms of implementation the GC variants require extra parameters (shadowed crown and ground reflectance) but this evidence does suggest that these kernels may be better equipped to describe the GO component of $\rho_{canopy}$ in a wider variety of cases (for the type of canopy examined here). At the very least the GC variants should be considered a viable alternative to the standard GO kernels.
5.4 Conclusion

The hypothesis that $\rho_{\text{canopy}}$ can be represented as a linear combination of volumetric and GO components, $\alpha$ and $\beta$, was tested by separating these components from BPMS-simulated $\rho_{\text{canopy}}$, and plotting their relationship with the respective linear model kernels, $k_{\text{vol}}$ and $k_{\text{GO}}$. Results from barley and wheat canopies show that there is generally a linear relationship between $\alpha$ and $k_{\text{vol}}$, which becomes stronger as the canopies develop. The values of $r$ for the regressions of $\alpha$ against $k_{\text{vol}}$ generally increase with $\theta$, and decrease with $\phi_{\text{row}}$ until the canopy no longer adheres to the assumptions used in the kernels exemplified by the 24\textsuperscript{th} June barley canopy (LAI of 3.19, but little green vegetation and lots of seed heads). This behaviour is likely to be due to an increase in the proportion of volumetric scattering caused by increasing path length (of incoming radiation) through the canopy.

Results show a much weaker relationship between $\beta$ and $k_{\text{GO}}$, than between $\alpha$ and $k_{\text{vol}}$. There is also greater variability in the values of $r$ in this case. The values of $r$ for $\beta$ against $k_{\text{GO}}$ tend to fall as the canopy develops and volumetric scattering increases at the expense of GO scattering. Also in contrast to $\alpha$, $r$ falls with $\theta$ in all cases except for the 24\textsuperscript{th} June barley canopy. There is little variation in correlation between $\beta$ and $k_{\text{GO}}$ with $\phi_{\text{row}}$, except (again) for the 24\textsuperscript{th} June barley canopy. Although results for $\alpha$ (in particular) and $\beta$ indicate that $\rho_{\text{canopy}}$ may be separated into a linear combination of volume and GO scattering components in some cases, it is clear that this separability will depend on canopy configuration. The canopies used here depart (deliberately) from those envisioned in the linear kernels (particularly the GO case): they are row-oriented, with non-spherical LAD and small, widely distributed scatterers rather than GO "envelopes". In particular, as the canopies develop, they resemble the idealised 'spheroids on sticks' assumption of the GO kernels less and less. The key issue is that $\rho_{\text{canopy}}$ can always be approximated (badly) by a linear combination of volumetric and GO components. However, results presented in this chapter illustrate that in cases where the canopy configuration more closely resembles that envisioned in the formulation of the kernels, the linear assumption is reasonable, particularly in the volumetric case. The barley and wheat canopies used for the simulation of $\rho_{\text{canopy}}$ in this chapter resemble the configuration envisioned in the volumetric kernels far more closely than that envisioned in the GO kernels, so it is not surprising that agreement between $k_{\text{vol}}$ and $\alpha$ is far higher than that between $k_{\text{GO}}$ and $\beta$. 

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The canopies used in this experiment were deliberately chosen to diverge from the assumptions of plane-parallel homogeneity and distinct crown-shape on which $k_{vol}$ and $k_{GO}$ respectively are based. This was done in order to explore the applicability of the kernels in cases where their assumptions are not met directly (which perhaps applies to most cover types). When the assumptions underlying the kernels are not met, the assumption that $\rho_{canopy}$ can be described as a linear combination of volumetric and GO scattering components tends to break down. These cases are listed below:

i) The canopy is very sparse, and there is almost no scattering from vegetation ($k_{vol}$ attempts to explain some GO scattering). This is seen in the variability (and general reduction) of $r$ with $k_{vol}$ in table 5.1e.

ii) The canopy is very dense, but the LAI is (relatively) low e.g. when the canopy reaches maturity and is largely stems and seed heads with little green leaf area (see variation of $r$ with $k_{vol}$ in table 5.1d).

iii) There is noticeable azimuthal variation in the vegetation density due to row planting patterns (assumption of azimuthal uniformity invalidated). This is true for $k_{GO}$ in the 24th June barley canopy case (table 5.2d). However, the large variation seen in the correlation between $k_{vol}$ and $\alpha$, and $k_{GO}$ and $\beta$ with $\theta_v$ is also a function of variation in $\phi_{row}$. As the canopy is seen across and along rows, the density of (viewed) vegetation changes significantly, causing variation in the amount of visible sunlit (and shaded) soil and vegetation (clumping). This is especially true for the barley canopy of 24th June. Figure 5.6 shows the large variation in sunlit leaf and soil with $\phi_{rows}$ at high $\theta_v$. The variation is not as pronounced for younger canopies or for lower $\theta_v$.

iv) Canopy LAD departs from the assumed spherical distribution (see figure 4.8) i.e. 23rd March wheat (see variability of $r$ values in table 5.1e).

v) Inappropriate kernel choices are made i.e. RossThick kernel when LAI is low (table 5.1a and e), or RossThin when LAI increases (table 5.1b-d). This is not true of $k_{GO}$ as the LiSparse kernel proved a better fit in nearly all circumstances (table 5.2). So, interestingly, the "wrong" kernel choice can in some cases provide a better fit to reflectance. This indicates some kernel combinations may be inherently more flexible than others, although any biophysical information contained in the model parameters in these cases should not be trusted.
Figure 5.6 Variation in sunlit leaf and soil, 24th June barley canopy, $\theta_l = 60^\circ$.

The factors listed above highlight the importance of interpretation when using model parameters derived from satellite and airborne reflectance measurements. It is preferable that a minimum of assumptions regarding the type and distribution of cover be made. However, results presented here suggest that the assumption of $\rho_{\text{canopy}}$ as a linear combination of volumetric and GO scattering components is not always true. If cover types do not conform to the approximations underlying the linear models, attempts to evaluate parameters such as LAI and shadow fraction should not be made. Conversely, the parameters may directly indicate regions of departure from the assumptions made in the linear models. In these cases it is still possible to derive integrated products such as albedo, but no conclusions should be drawn regarding surface biophysical parameters. Constraints may be applied in these cases to ensure adherence to physical principles such as energy conservation (see appendix 1). The next stage of analysis is to examine more closely the information content of volumetric and GO model parameters inverted against simulated $\rho_{\text{canopy}}$. It is important to understand whether it may be possible to retrieve biophysical information from the inverted model parameters (and if so, what sort) or whether the kernels should only ever be used for generating integrated products such as albedo, or predicting reflectance behaviour (Roy et al., 2001).
Evidence presented in chapters 4 and 5 supports the first hypothesis of section 4.2 i.e. that $\rho_{\text{canopy}}$ can (in general) be modelled as a linear combination of volumetric and GO kernels describing the (angular) variation of the separate components. However as the structure of the canopy departs from the assumptions made in the formulation of the kernels this hypothesis tends to break down. For sparse canopies $k_{\text{vol}}$ can apparently explain a significant part of the variation seen in $\rho_{\text{canopy}}$ even though there is likely to be very little volumetric scattering in these cases (reflected in the high values of the correlation coefficient, $r$, seen in table 5.1). Likewise, $k_{\text{GO}}$ generally seems to explain variations in $\rho_{\text{canopy}}$ for the dense canopies when the scattering will be predominantly volumetric. This poses the question of whether the kernels can be said to be acting independently of each other. If not, attributing meaning to derived biophysical parameters will be much more difficult as the model parameters will be coupled in some way.

The issue of information in linear BRDF model parameters will be addressed in the subsequent section with reference to the second hypothesis of section 4.2, namely that the kernels describing the volumetric and GO scattering components of $\rho_{\text{canopy}}$ act independently of each other. If this hypothesis is true, then the volumetric component of $\rho_{\text{canopy}}$ should be adequately modelled by the volumetric kernel alone and the GO component of $\rho_{\text{canopy}}$ should be described solely by the GO kernel. This implies that no part of the variation of either component should be explained by the other kernel. In this case the components are separable and orthogonal. In practical cases where the models do not satisfactorily describe the BRDF, and assuming that angular sampling is reasonable (Lucht and Lewis (2000) have shown that poor angular sampling can severely affect the kernels' ability to fit BRDF), it is assumed that the basic kernel shapes are inadequate to describe the primary reflectance variations or that the assumptions underlying the kernels may not be fully met. The possibility that there may be secondary (and higher) components of the volumetric or GO components of the scattered reflectance field which may be described in part by the other kernel is not considered.

Kernel-driven models are specifically designed to cope with spatially heterogeneous surfaces where both volume and GO scattering may be present due to the
variety of cover types that may be contained in a single pixel (Wanner et al., 1995). This permits inversion against moderate resolution reflectance data where heterogeneity can otherwise present severe problems. An example of this type of surface might be sparse woodland interspersed with grassland, where the shadows cast by the tree crowns conform to the GO model, whilst scattering within the tree crowns and from the grass is likely to be predominantly volumetric. Such a surface suggests that a continuum of the two scattering components exists, potentially operating at different scales (Wanner et al., 1997). Is it reasonable in such a case to assume that all variation in each of the two components can be completely described by the respective kernels? If not, it is likely that the model parameters cannot be ascribed the direct physical meaning given in their formulation (see equations 4.3 and 4.4), but rather that the parameters are coupled in some sense.

If we wish to invert the linear models against reflectance data in order to derive biophysical information it is essential to understand the physical meaning of the model parameters, whether the parameters are coupled, and if so, in what sense. As an example, consider equation 4.2: knowing \( P(\theta, \theta_s, \phi) \), \( G \) and \( G' \), \( \mu \) and \( \mu' \), is it possible to invert LAI explicitly from \( \rho_{\text{canopy}} \), or will LAI and \( \rho_{\text{leaf}} \) be coupled in some way? If so, then to derive LAI by inverting a kernel-driven model against measured \( \rho_{\text{canopy}} \) would require knowledge of specific \( \rho_{\text{leaf}} \) for the observed canopy. The following section investigates the possibility that \( \rho_{\text{canopy}} \) cannot necessarily be separated into volumetric and GO scattering components and that some part of each component may actually be described by the other kernel. In addition, spectral variation of the angular kernels is discussed.
6.2 Method

If the linear relationships between $k_{vol}$ and $\alpha$ and $k_{GO}$ and $\beta$ described in equations 4.3 and 4.4, and demonstrated experimentally in chapter 5, are substituted into equation 4.1, a simplified expression for $\rho_{canopy}$ is obtained in terms of the coefficients of the linear relationships presented in tables 5.2 and 5.3 ($a_{vol,GO}$ and $b_{vol,GO}$):

$$\rho_{canopy} = \left( \rho_{leaf} \frac{b_{vol}}{a_{vol}} + \rho_{soil} \frac{b_{GO}}{a_{GO}} \right) + \rho_{leaf} \frac{k_{vol}}{a_{vol}} + \rho_{soil} \frac{k_{GO}}{a_{GO}}$$

Equation 6.1 contains a purely volumetric term, a purely GO term and a term comprising $\rho_{leaf}$ and $\rho_{soil}$ multiplied by the ratio of $b$ to $a$ (slope over intercept) from equations 4.3 and 4.4. If equation 6.1 is compared with the general expression for a full kernel-driven model (equation 2.27) it can be seen that (except for the role $f_{iso}$ has in taking up the multiple scattering component) there is a direct equivalence between the model parameters i.e.

$$f_{iso} = \left( \rho_{leaf} \frac{b_{vol}}{a_{vol}} + \rho_{soil} \frac{b_{GO}}{a_{GO}} \right)$$  \hspace{1cm} 6.2a$$

$$f_{vol} = \frac{\rho_{leaf}}{a_{vol}}$$  \hspace{1cm} 6.2b$$

$$f_{GO} = \frac{\rho_{soil}}{a_{GO}}$$  \hspace{1cm} 6.2c$$

where $f_{iso,GO,vol}$ are the model parameters (equivalent to the kernel weightings as described in section 2.5.4.1, ignoring multiple scattering effects). We can now obtain estimates of the volumetric and GO parameters $f_{vol}$ and $f_{GO}$ from two directions:

1. From the values of $a_{vol}$ and $a_{GO}$ in tables 5.1 and 5.2 in combination with appropriate spectral estimates of $\rho_{leaf}$ and $\rho_{soil}$, using the relationships in equations 6.2b and 6.2c.

2. From inverting a full linear kernel-driven model (as expressed in equation 2.27) against $\rho_{canopy}$ calculated from substitution of $a_{vol,GO}$ and $b_{vol,GO}$ back into equation 6.1.
If the separate (single) scattering components of $\rho_{\text{canopy}}$ can be modelled by isolating the purely geometric parameters controlling them (i.e. $f_{\text{vol}}$ and $f_{\text{GO}}$, all other factors being equal) by assuming that $\rho_{\text{canopy}}$ can be represented as a linear combination of volumetric and GO components $\alpha$ and $\beta$, then clearly the same values of $f_{\text{vol}}$ and $f_{\text{GO}}$ should be obtained from method 1 above as from method 2. This is illustrated schematically in figure 6.1. If there are significant differences between the values of $f_{\text{vol}}$ and $f_{\text{GO}}$ derived from $a_{\text{vol,GO}}$ and $b_{\text{vol,GO}}$ and those obtained through full model inversion then we must conclude that the volumetric and GO kernels are not entirely separable i.e. hypothesis two of section 4.2 is false, and, as a result, the retrieval of uncoupled biophysical parameters from linear model inversions may not be possible. In this case it may be possible to identify coupled parameter relationships which might be inverted, but the nature of the coupling will need to be understood. This has important consequences for the operational use of linear kernel-driven BRDF models: without a clear understanding of the physical meaning of model parameters inverted from reflectance data, they are likely to be wrongly used and interpreted.

![Diagram](image)

**Figure 6.1** Estimates of model parameters $f_{\text{iso}}$, $f_{\text{vol}}$ and $k_{\text{GO}}$ (spectrally varying)

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1. Estimates of $a_{\text{vol,GO}}$ and $b_{\text{vol,GO}}$ derived from regression analysis, plus substitution of suitable $\rho_{\text{leaf,soil}}$

2. Inversion of full linear kernel-driven model against $\rho_{\text{canopy}}$ derived using $a_{\text{vol,GO}}$ and $b_{\text{vol,GO}}$ plus suitable $\rho_{\text{leaf,soil}}$
6.3 Results

The values of $a_{\text{vol},G0}$ and $b_{\text{vol},G0}$ presented in tables 5.1 and 5.2 were used in conjunction with suitable values of $\rho_{\text{leaf}}$ and $\rho_{\text{soil}}$ to calculate (spectrally varying) values of model parameters $f_{G0}$ and $f_{\text{vol}}$ according to equations 6.2b and c. The $\rho_{\text{leaf}}$ and $\rho_{\text{soil}}$ spectra used are shown in figure 6.2. These spectra were obtained during the field campaign described in chapter 3 using the PSII radiometer. Leaf spectra recorded in this manner (with leaves still attached to the plants) may not be a totally accurate measure of leaf reflectance as some radiation impinging on the leaf is lost via transmission through the lower surface of the leaf, while some reflected radiation will not fall within the instrument IFOV. Laboratory measurements are generally made using an integrating sphere, in order to ensure all incident radiation is recorded. However, in these experiments the absolute values of reflectance are not so important, it is the behaviour across the spectrum that is of interest. From figure 6.2, the values of leaf are higher in the NIR than might be expected.

At the same time as values of $f_{G0}$ and $f_{\text{vol}}$ are derived via the regression relationships of chapter 5, a full kernel-driven model of the type described in equation 2.27 was inverted against values of $\rho_{\text{canopy}}$ calculated by substituting the parameters $a_{\text{vol},G0}$

![Figure 6.2](image.png)

**Figure 6.2** $\rho_{\text{leaf}}$ and $\rho_{\text{soil}}$ used in BPMS $\rho_{\text{canopy}}$ simulations
b_{vol,GO}, \rho_{leaf} and \rho_{soil} into equation 6.1. These spectrally varying f_{GO} and f_{vol} are presented alongside the values of f_{GO} and f_{vol} calculated directly from tabulated values of a_{vol} and a_{GO} (plus \rho_{leaf} and \rho_{soil}) via equations 6.2b and c. Figures 6.3 and 6.4 show the comparisons between the two sets of model parameters. Results are shown for the isotropic, RossThick and LiSparse kernel combination (figure 6.3) as well as the isotropic, RossThin, LiDense combination (figure 6.4). In figures 6.3 and 6.4 the parameters derived through the use of the derived a_{vol,GO} and b_{vol,GO} values are referred to as “BPMS” (or “BPMS-derived”) parameters, and those through the inversion of a full linear model as “inverted”. These distinctions are artificial as both sets of parameters are derived from BPMS simulations and both are obtained by inversion (although in different senses), but they need to be distinguished in subsequent discussions.
Figure 6.3 Comparison of isotropic, volumetric (RossThick) and GO (LiSparse) parameters derived from BPMS simulations and inversion of a full linear model.

a) barley - 18th April

b) barley - 13th May
c) barley - 4\textsuperscript{th} June

d) barley - 24\textsuperscript{th} June
e) wheat - 23rd March

f) wheat - 23rd April
Figure 6.4 Comparison of isotropic, volumetric (RossThin) and GO (LiDense) parameters derived from BPMS simulations and inversion of a full linear model.

(a) barley - 18th April

(b) barley - 13th May
c) barley - 4th June

d) barley - 24th June
c) wheat - 23rd March

f) wheat - 23rd April
6.4 Discussion

Figures 6.3 and 6.4 show comparisons of the isotropic, volumetric and GO parameters ($f_{iso}$, $f_{vol}$ and $f_{GO}$) obtained from:

i) Substituting values of $a_{vol,GO}$ and $b_{vol,GO}$ (derived from relating the volumetric and GO components of BPMS-simulated $\rho_{canopy}$, $\alpha$ and $\beta$, to $k_{vol}$ and $k_{GO}$) along with selected $\rho_{leaf}$ and $\rho_{soil}$ back into equations 6.2a-c (in essence 'calibrating' the kernels to each canopy under consideration).

ii) Inversion of a full linear kernel-driven BRDF model against values of $\rho_{canopy}$ derived by substituting values of $a_{vol,GO}$, $b_{vol,GO}$, $\rho_{leaf}$ and $\rho_{soil}$ into equation 6.1. Inversion in this case is performed fitting three kernels (isotropic, volumetric, GO) to the BPMS-simulated values of $\rho_{canopy}$ by the standard linear (matrix) inversion methods described in 2.4.1. Inversion is performed against values of $\rho_{canopy}$ simulated at all $\theta_v$ (-70° to 70°), $\theta_i$ (0°, 30°, 60°) and $\phi_{row}$ (0°, 45°, 90°).

The aim of this is to establish what information might be contained within the model parameters, $f_{iso}$, $f_{vol}$ and $f_{GO}$. This has implications for how the inverted kernel-driven model parameters are used in practice and what information they can be expected to yield. Results for each canopy are discussed separately in turn in sections 6.4.1 to 6.4.6. In general terms however, the correlation between the two sets of parameters is very high as would be expected (values of the correlation coefficient higher than 0.95 in all cases). The main discrepancy is a tendency for the inverted GO parameter to 'flip' negative sometimes, in a mirror image of the BPMS-derived value. This is discussed below.

6.4.1 Barley canopy, 18th April

For the isotropic, RossThick, LiSparse kernel combination the two sets of parameters agree well, particularly in the visible, with some divergence in the near IR. Both estimates of $f_{iso}$ are relatively small in magnitude and spectrally ‘flat’, with a small rise in the near IR. The largest spectral variation by far is in $f_{vol}$. The volumetric
component of \( \rho_{\text{canopy}} \), \( \alpha \), is proportional to the \( 1-e^{-L_1} \) term in equation 4.2, but the spectral shape indicates that \( \alpha \) is also a function of \( \rho_{\text{leaf}} \) (the leaf-scattering phase function \( P(\theta_1, \theta_2, \phi) \) and the leaf projection function \( G(\theta_1, \theta_2, \phi) \) are both geometric terms i.e. not a function of \( \lambda \)). Both estimates of \( f_{\text{vol}} \) exhibit spectral variation: very low reflectance at visible wavelengths due to chlorophyll absorption including a peak in the visible green centred at around 560 nm, and a large increase of reflectance across the red edge from the visible to the near IR wavelength regions at around 700-800 nm. The form of \( f_{\text{vol}} \) in figures 6.3 and 6.4 follows exactly the form of \( \rho_{\text{leaf}} \) shown in figure 6.2. This is unsurprising as \( \alpha \) is defined as the component of \( \rho_{\text{canopy}} \) due to scattering from vegetation (equation 4.3). It is independent of \( \rho_{\text{leaf}} \) (a geometric parameter only) but the insertion of the spectra described above re-introduces this dependence. The degree of correspondence of \( f_{\text{vol}} \) to \( \rho_{\text{leaf}} \) effectively defines the degree of dominance of the volumetric component of \( \rho_{\text{canopy}} \) by scattering from vegetation, and is a further indicator of the fact that \( \rho_{\text{canopy}} \) can be separated into volumetric and GO components.

In contrast \( f_{\text{GO}} \), controlled by the amount of visible sunlit and shadowed soil, shows little spectral variation (compared to the assumed soil spectrum, \( \rho_{\text{soil}} \), of figure 6.2). The relation between the spectral variations of \( f_{\text{vol}} \) and \( f_{\text{GO}} \) and the spectral components of \( \rho_{\text{canopy}} \), \( \rho_{\text{leaf}} \) and \( \rho_{\text{soil}} \), suggest that model parameter estimates of this sort may well be useful for spectral discrimination of cover types i.e. classification. In such an application, the absolute values of the parameters are unimportant but the relative magnitudes could be used to map spatial distribution of volumetric and GO scattering components (equivalent to vegetated and non-vegetated regions). This is of consequence in applications where estimates of total vegetation amount are required, such as in analysis of carbon budgets and net primary productivity.

The isotropic, RossThin and LiDense kernels (figure 6.4a) are almost an order of magnitude smaller than for the previous case, with \( k_{\text{vol}} \) barely rising to 1, as opposed to around 5.5 above. Values of \( f_{\text{vol}} \) still agree within a few percent but there are discrepancies between the BPMS-derived and inverted isotropic parameters in the visible region, with the inverted parameter showing a distinct “vegetation-like” rise in magnitude from the visible to the near IR. The same is true of the inverted \( f_{\text{GO}} \), unlike the BPMS-derived \( f_{\text{GO}} \), which closely resembles the \( \rho_{\text{soil}} \) of figure 5.2. This suggests that perhaps \( f_{\text{iso}} \) and \( f_{\text{GO}} \) are describing some of the scattering due to vegetation that is not being explained
by $f_{vol}$. This would also explain why the contrast between $f_{iso}$, $f_{GO}$ and $f_{vol}$ in the near IR is not as great as would be expected. This combination of kernels is not as effective at describing $\rho_{canopy}$ as the previous one, although in this case $f_{GO}$ follows $\rho_{soil}$ more closely than in the previous case. As in chapter 5 this adds further weight to the choice of the isotropic, RossThick and LiSparse kernel combination for inversion against reflectance data where no a priori knowledge of cover type is assumed (Hu et al., 1997; Wanner et al., 1997).

6.4.2 Barley canopy, 13th May

The trends in the inverted isotropic, RossThick plus LiSparse model parameters for the 13th May barley canopy are similar to those of 18th April. Agreement in magnitude between the BPMS-derived and inverted parameters is very good, particularly $f_{iso}$ (greater than 95%). Notable differences are the increased magnitude, particularly of the volumetric parameter (maximum of nearly 8 as opposed to 5.5 for 18th April), the 20% increase in magnitude of the BPMS-derived volumetric parameter over the inverted volumetric parameter in the near IR, and the clear rise of the isotropic parameters across the red edge. This last factor again suggests that some of the variation due to volume scattering may be being taken up by $f_{iso}$. Both the $f_{GO}$ are spectrally flat and very small in magnitude.

The isotropic, RossThin LiDense parameters for the 13th May are quite different (6.4b). The magnitudes are again much lower than for the isotropic, RossThick LiSparse combination, as was seen for the 18th April canopy (compare figures 6.3a and 6.4a). The $f_{iso}$ show the greatest spectral variation, increasingly resembling the volumetric parameter in figure 6.3. In addition, the BPMS-derived GO parameter, still relatively flat, differs markedly from the inverted GO parameter, which is much closer in appearance to the inverted volumetric parameter. These observations suggest that if non-optimal kernel combinations are selected, the information content of the model parameters becomes increasingly difficult to explain.
6.4.3 Barley canopy, 4\textsuperscript{th} June

The magnitude of both sets of parameters in the isotropic, RossThick, LiSparse combination increases again (figure 6.3c) up to a maximum of between 8.5 and 11.5 for both $f_{iso}$. Both isotropic parameters again appear to explain some of the spectral variation due to scattering from vegetation. The inverted values of $f_{GO}$ also display a slight increase with wavelength, but this is not true for the BPMS-derived $k_{GO}$. This may indicate that the parameter space of the full linear model inversion is larger than that for the parameter values derived using the estimates of $a_{vol,GO}$ and $b_{vol,GO}$, allowing spectral components of volumetric scattering to be spread across all three parameters rather than confined to one. The results presented in section 5.3 illustrate that in some cases the relationship between the GO component of $\rho_{canopy}$, $\beta$, and the GO kernels is not clear. It is predictable in these cases that the inverted model parameters are likely to describe a combination of both volumetric and GO components of $\rho_{canopy}$. Apart from the BPMS-derived GO parameter, all the parameters in figure 6.4c (isotropic, RossThin, LiDense) except the BPMS-derived GO parameter show a sharp rise in magnitude across the red edge suggesting that the volumetric component increasingly dominates $\rho_{canopy}$ as the canopy develops.

6.4.4 Barley canopy, 24\textsuperscript{th} June

Results from this canopy are different again, as the canopy has matured and begun to senesce. The BPMS-derived values of $f_{vol}$ still display the strong vegetation-like shape, but, in contrast to previous results, the inverted parameters do not follow this pattern at all and are very much lower in magnitude. The inverted $f_{iso}$ is the only parameter which rises significantly above zero. It is perhaps ill-advised to attempt to explain the variations in this case as the canopy is now divergent from the assumptions made in the formulation of either the volumetric or GO kernels. It has already been shown that this divergence results in the inability of the linear kernel-driven models to describe the directional and spectral features of $\rho_{canopy}$ adequately (see section 5.3.2). This inability is strongly apparent in the results of the isotropic + RossThin + LiDense kernel combination for the same date (figure 6.4d). The BPMS-derived isotropic parameter in this case has become virtually a negative reflection about the x-axis of the BPMS-derived volumetric parameter. The other parameters generally follow the same shapes as in the previous case.
6.4.5 Wheat canopy, 23rd March

Results from the isotropic + RossThick + LiSparse combination for the wheat canopy of March 23rd (figure 6.3e) show a number of differences from the results of the barley canopies. The two isotropic parameters agree closely but are similar in shape and magnitude to the volumetric parameter of the barley canopies of 18th April and 13th May. However, both $f_{vol}$ in this case are negative, with the BPMS-derived estimate of $f_{vol}$ being a virtual reflection of both $f_{iso}$ about the x-axis. This suggests the volumetric parameter is over-compensating for the vegetation element contained in the isotropic parameter. All other parameters are close to zero. Similarly, the isotropic + RossThin + LiDense combination has both isotropic parameters following closely the shape of $\rho_{leaf}$ (in a similar manner to the behaviour of the volumetric parameter in the barley cases). This canopy is very sparse (LAI = 0.08) and the volume scattering component has been shown to be small (figure 4.5). This further illustrates how scattering originating from one component of $\rho_{canopy}$ may be 'taken up' by another parameter if the assumptions underlying the kernels are not met and/or an unsuitable combination of kernels is selected. The BPMS-derived GO parameter is similar in shape (and relative magnitude compared with $f_{vol}$) to $\rho_{soil}$ which is less surprising, as it might be expected that $\rho_{canopy}$ be dominated by $\rho_{soil}$ with so little vegetation being present.

6.4.6 Wheat canopy, 23rd April

The behaviour of the isotropic, RossThick and LiSparse parameters for this canopy are similar to those of the previous wheat case, with an exaggeration in magnitude. Both isotropic parameters are (relatively) high and similar in shape to $\rho_{leaf}$, although agreement between the two is less than for the previous wheat canopy, particularly in the near IR where the BPMS-derived parameter is significantly higher than the inverted parameter. As the volumetric component of $\rho_{canopy}$ increases from 23rd March to 23rd April, differences between the two sets of parameters become more apparent. The BPMS-derived and inverted volumetric parameters are both negative as in the 23rd March case but even more so, suggesting over-compensation during inversion. In terms of shape and magnitude the inverted estimates of the GO parameter lie somewhere between the inverted isotropic and the BPMS-derived GO parameter, which is close to zero across all
wavelengths. This is due to the structure of the wheat canopy. It has been shown that this canopy has a somewhat different structure from the other canopies in this experiment, with a strongly erectophile LAD (figure 4.8). If $\theta_v$ departs significantly from nadir, very little soil will be visible to the viewer (see figure 4.7). In this case, scattering from the canopy (under the assumption of single scattering interactions only) will be dominated by the component originating from the vegetation alone.

Results from the isotropic + RossThin + LiDense kernel combination (figure 6.4f) are even more variable than for the various barley canopies. Both isotropic parameters are similar in shape to the parameters inverted from the isotropic + RossThick + LiSparse kernel combination for this canopy (figure 6.3f) with the BPMS-derived parameter being similar in magnitude and the inverted isotropic parameter being significantly lower. The GO parameters also show similar behaviour but with the BPMS GO parameter rising above zero in this case. The volumetric parameters in both cases are negative.

### 6.4.7 Summary

Results show that there is good agreement in some cases between the two sets of model parameters - those derived from inversion of a full kernel-driven model against $\rho_{canopy}$ and those derived from regression of the BPMS-derived reflectance components $\alpha$ and $\beta$ against the separate volumetric and GO kernels. However, agreement is not always good and for some canopies the two parameter sets differ markedly, notably when the BPMS parameters turn negative. Table 6.1 shows values of $r^2$ for the two sets of $f_{iso}$, $f_{vol}$ and $f_{GO}$ parameters. In each case, the values are given from the isotropic + RossThick + LiSparse kernel combination and the isotropic + RossThin + LiDense kernel combination.

As the barley canopy develops, the parameters (including the isotropic parameter, $f_{iso}$) increasingly resemble $\rho_{leaf}$. This indicates the parameters are not limited to dependence on purely geometric terms as intended (if this were the case, we would expect $f_{vol}$ to resemble leaf, $f_{GO}$ to resemble soil, and $f_{iso}$ to be spectrally flat). The relative magnitude of the parameters generally varies as expected, with the volumetric parameter (and to an extent the isotropic parameter) increasing with LAI relative to the GO parameter but at the expense of increased coupling. As the canopy departs from
assumptions underlying the kernels (geometrically and radiometrically) the parameters become negative, or become coupled. This is most obvious in the case of the wheat canopy of 23\textsuperscript{rd} April, which has a strongly erectophile LAD. Discrepancies between the two sets of parameters also become more apparent in the barley canopy as it develops, particularly for the 24\textsuperscript{th} June case (figures 6.3d and 6.4d) which least resembles the assumptions made in the kernel-driven models. In the case of the isotropic + RossThick + LiSparse kernel combination, the BPMS isotropic parameter is far larger then the corresponding inverted isotropic parameter, in fact larger than all other parameters by far. For the isotropic + RossThin + LiDense kernel combination, the BPMS isotropic parameter turns negative, indicating an unsuitable choice of kernels.

Table 6.1 $r^2$ values for BPMS-derived against inverted values of $f_{iso}$, $f_{vol}$ and $f_{GO}$.

<table>
<thead>
<tr>
<th>Canopy</th>
<th>$f_{iso}$</th>
<th>$f_{vol}$</th>
<th>$f_{GO}$</th>
<th>$f_{iso}$</th>
<th>$f_{vol}$</th>
<th>$f_{GO}$</th>
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<td>barley 18/4</td>
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<td>0.99</td>
<td>0.95</td>
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<td>0.99</td>
<td>0.95</td>
</tr>
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<td>0.99</td>
<td>0.94</td>
<td>0.99</td>
<td>0.98</td>
<td>0.94</td>
</tr>
<tr>
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<td>0.96</td>
<td>-0.99</td>
<td>-0.99</td>
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</tr>
<tr>
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<td>0.99</td>
<td>-0.99</td>
<td>0.95</td>
</tr>
<tr>
<td>wheat 23/4</td>
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<td>0.98</td>
<td>0.95</td>
<td>0.99</td>
<td>-0.99</td>
<td>0.95</td>
</tr>
</tbody>
</table>

6.5 Implications of coupling between model parameters

It is clear from results presented above (and previously) that the volumetric and GO components of $\rho_{canopy}$ are separable in many cases. However, it is also clear that as a canopy develops and the magnitude of the respective volumetric and GO parameters increases (particularly $k_{vol}$), observed behaviour departs from that which might be expected if the components were completely separable. The relationships between $\alpha$ and $k_{vol}$ and $\beta$ and $k_{GO}$ presented in chapter 5 show that a proportion of both the volumetric and GO components of $\rho_{canopy}$ are not described by the corresponding kernel: the relationships are not perfectly linear by any means. There is a possibility that a residual
part of the volumetric component, $\alpha$, not described by $k_{vol}$ may be described by $k_{GO}$, and conversely, some proportion of the GO component, $\beta$, may be explained by $k_{vol}$. As an example, the rise of the volumetric parameter across the red edge for the barley canopies of 13th May and 4th June and the wheat canopy of 23rd April are coupled to a similar increase in the GO parameter (figures 6.3 and 6.4). Clearly $\alpha$ is not completely described by $k_{vol}$; the GO parameter, $f_{GO}$, also contains information related to $\alpha$. From equation 4.2, for a given $(\theta_1, \theta_2, \phi)$, $\alpha$ is proportional to $(1-e^{-1LAi})$ (all other terms in equation 4.2 being purely dependent on $\theta_1, \theta_2, \phi$). From equation 4.2 it can also be seen that the spectral variation of the volumetric component of $p_{canopy}$ is controlled by $\rho_{leaf}$. In all cases, the accuracy with which the kernels can describe $p_{canopy}$ will be dependent on angular sampling (Lucht and Lewis, 2000). In the experiments presented in this thesis $p_{canopy}$ can be simulated at arbitrary $(\theta_1, \theta_2, \phi)$ as required and consequently angular sampling is not an issue. However, in practice the impact of poor angular sampling will compete with (and possibly outweigh) the coupling of volumetric and GO parameters to reduce the kernels’ ability to describe $p_{canopy}$.

Having shown in chapter 5 that it is possible (in the main) to isolate the geometric factors controlling $p_{canopy}$ through wavelength-independent simulations, the results of the previous section present spectrally varying estimates of model parameters. It is immediately obvious from figures 6.3 and 6.4 that $\alpha$ is proportional to $\rho_{leaf}$. This implies that the geometric and spectral parts of the volumetric component of $p_{canopy}$ are linked. The question is whether they are inextricably linked. If so, it may not be possible to invert parameters such as LAI directly from reflectance data as the geometric factors are likely to be coupled to spectral information (i.e. $\rho_{leaf}$). In order to separate LAI from a coupled $\rho_{leaf} (1-e^{-1LAi})$ term, an estimate of $\rho_{leaf}$ would be needed. A requirement for ancillary data of this sort potentially limits the use of inverted biophysical parameter information unless: (i) $\rho_{leaf}$ data are available; or (ii) a priori assumptions are made regarding the cover types over which such models are applied. Option (i) is generally not practical if specific $\rho_{leaf}$ data are required, simply because of the variety of vegetation types and the scarcity of high quality field-measured spectral reflectance data. Option (ii) is not desirable given that one purpose of the linear kernel-driven approach is to allow application of models to reflectance data of arbitrary cover types, at a range of scales (neglecting adjacency effects). In relation to (i) above it should be noted however that it is clear that most (if not
all) green $\rho_{leaf}$ spectra share many attributes, namely a maxima of reflectance at visible green wavelengths, a minima in the visible red, and a sharp rise across the NIR region. The possibility that this can be exploited, in a manner similar to the generalisation of BRDF shape made in the linear kernel-driven models, is explored in chapter 7. At any rate, evidence presented here and in chapter 4 demonstrates that inverted parameters from reflectance data must be interpreted carefully if they are to be used directly (rather than for deriving integrated parameters such as albedo, or for classification).

If such parameter coupling is significant, then we might expect that the data used in chapter 4 to explore the relationships between i) $k_{vol}$ and $\alpha$, and ii) $k_{GO}$ and $\beta$, would show two distinct dimensions of information related to the two components of scattering behaviour. These data are the (supposedly) separate volumetric and GO scattering components of BPMS-simulated $\rho_{canopy}$, $\alpha$ and $\beta$. If canopy information is not coupled, $\alpha$ will describe only volumetric scattering, and $\beta$ will describe only GO scattering, as defined in equation 4.1. If there is coupling however, each component of $\rho_{canopy}$ will contain information related to the other. In order to examine this possibility, principal component analysis (PCA) was performed on the respective combinations of $\alpha$ and $k_{vol}$ and $\beta$ and $k_{GO}$. PCA allows a set of correlated observations to be transformed to a set of uncorrelated (principal) components (pcs) by calculating the eigenvectors and eigenvalues of the variance-covariance matrix of observations (Jolliffe, 1986). The percent variance in the data described by each pc is simply the corresponding eigenvalue, scaled by the sum of all eigenvalues. In this case, the magnitudes of the first two principal components will indicate the relative importance of the scattering components. If $\alpha$ describes only the volumetric component of canopy scattering, it would be expected that $pc1$, the first principle component, would be completely dominant, with $pc2$ having a far lower magnitude. The same argument applies to $\beta$ and $k_{GO}$. If there is significant coupling in either case however, it would be expected that the magnitude of $pc1$ and $pc2$ might be comparable. Results of the PCA are presented in figure 6.5. Results are presented for the simulations carried out with $\phi_{row} = 0^\circ$, for all three values of $\theta$, i.e. $0^\circ$, $30^\circ$, and $60^\circ$.

The main feature of the results presented in figure 6.5 is that in all cases the first principal component is always larger than the second. This indicates that in each case there is a "dominant" component to the observed variance in the data. This is particularly true for the volumetric component of the early barley canopies, where $pc1$ of the
volumetric components (represented by the RossThick of RossThin kernels) rises as high as 99% (hence pc2 = 1%). In these cases nearly all the variance in $\alpha$ is explained by $k_{vol}$, and it is safe to assume that coupling is minimal. The case for $\beta$ is not quite so clear cut, with pc1 for the various $k_{GO}$ falling to between 60% and 70% in many cases, and down to almost 50% for the 23rd April wheat canopy. In this case there is significant variation in $\beta$ which is not being explained by $k_{GO}$. This supports the results presented in section 5.3 where the relationship between $\beta$ and $k_{GO}$ is not demonstrably linear as was the case for $\alpha$ and $k_{vol}$.

A second feature of figure 6.5 is the variation in the magnitude of the principal components with $\theta$. For the 18th April barley canopy, pc1 for the RossThick kernel starts at 85% for $\theta_i = 0^\circ$, rises to 96% for $\theta_i = 30^\circ$, and again to 98% at $\theta_i = 60^\circ$. There is even more variability for the various $k_{GO}$. The respective pc1s are virtually identical for $\theta_i = 0^\circ$ at 98%, except for the LiSparse kernel, where pc1 = 85%. For $\theta_i = 30^\circ$ there is a variability between the kernels in the magnitude of pc1 of around 20%, and by $\theta_i = 60^\circ$, they have fallen again to around 70%. This is the opposite trend to that observed for $\alpha$. 

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Figure 6.5 Principal component analysis of the separate $\alpha$ and $\beta$ components of $\rho_{\text{canopy}}$ for barley (four dates) and wheat (two dates).

a) barley - 18\textsuperscript{th} April

b) barley - 13\textsuperscript{th} May
c) barley - 4th June

d) barley - 24th June
c) wheat - 23\textsuperscript{rd} March

f) wheat - 23\textsuperscript{rd} April
The trends observed in figure 6.5 of both the magnitude of \( p_{c1} \) for \( \alpha \) and \( \beta \), and the variability with \( \theta_i \), are broadly similar for all the canopies under investigation. The major differences lie in the spread of points, with the more developed canopies having lower values of \( p_{c1} \) (and correspondingly higher \( p_{c2} \)). For the 23\(^{rd}\) March wheat canopy where very little vegetation is present, \( p_{c1} \) and \( p_{c2} \) of \( \alpha \) are relatively close, implying that there is no dominant "dimension" of the data to be explained by \( k_{vol} \). This agrees with the results presented in section 5.2.

For nearly all canopies the volumetric component has lower \( p_{c1} \) for \( \theta_i = 0^\circ \) than the GO component, and higher \( p_{c1} \) for \( \theta_i = 60^\circ \). In all cases except the barley canopy of 18\(^{th}\) April, \( \alpha \) is better described by the RossThick kernel. For \( \beta \) there is considerable variation with \( \theta_i \), within each canopy, but from one canopy to the next the pattern is the same: \( p_{c1} \) of \( \beta \) starts high for all kernels except LiSparse, then falls for \( \theta_i = 30^\circ \), where in all cases the LiDense canopy explains the most variance; \( p_{c1} \) falls again to \( \theta_i = 60^\circ \) where the LiSparse kernel performs the best. The consistency from one case to another suggests that the choice of kernel is more important than the variability of the data.

Conclusions to be drawn from the results presented above are simply that in most cases there is good reason to believe that \( p_{canopy} \) can be separated into volumetric and GO components. The caveat is that under certain where either the assumptions of the kernels are not met (as is the case in these experiments) or an unsuitable choice of kernels is used, this is not necessarily the case and care must be taken. In the canopies studied here the volumetric component tends to dominate \( p_{canopy} \), except in cases where the canopy is extremely sparse. The RossThick kernel tends to explain most variance in the volumetric component of \( p_{canopy} \), while the LiSparse kernel explains most variance in the GO component. The results for the GO kernels are less conclusive than those for the volumetric kernels.

The RossThick LiSparse kernel combination has been chosen for operational use as it appears to be the best at describing reflectance irrespective of surface, allowing it to be applied without \textit{a priori} knowledge of cover type. However this disguises the fact that over cover types where the assumptions underlying the kernels are not met, the RMSE of fit may not be significantly worse, yet the inverted model parameters are likely to have some very different, coupled meaning.
New techniques are being developed to alleviate this situation. Strugnell and Lucht (2000) have implemented a LUT relating land cover classes to field-measured BRDF shapes. The shapes of these measured class “archetypes” - BRDFs representative of each land cover class, are used to constrain the inversion of linear BRDF models against measured data. The assumption is made that BRDFs of cover types lying within a particular class will typically be closely related in shape with intra-class differences being one of magnitude rather than shape. By contrast, whilst unrelated cover types may have very similar spectral reflectances, their respective BRDFs will tend to differ as the underlying structure of the cover types is likely to be different. This use of existing knowledge of BRDF shapes of different cover types may be one way in which to inform the inversion of biophysical parameter information from linear models such that the most (physically) appropriate kernel combination is selected wherever possible. This method has been implemented for the initial surface reflectance and albedo products from MODIS. This so-called "magnitude inversion" method is used where insufficient angular samples of reflectance are available over a given 16-day period to permit a full inversion (the uncertainty is reflected in the associated QA information). A modification to the method of selecting appropriate kernel combinations for production of albedo where sufficient angular samples are available has recently been proposed. Gao et al. (2001) use least variance of white-sky albedo (bihemispherical reflectance) to select kernel combinations, rather than conventional least-squares fitting as proposed previously. Least variance of white-sky albedo appears to be a more effective way of selecting kernel combinations than RMSE, particularly when angular sampling is non-optimal which it will be in many situations. White-sky albedo also has the advantage that, as an integral of directional reflectance over the viewing and illumination hemisphere rather than an angular measure, it is an intrinsic surface property. Variance of observed white-sky albedo is a function of measurement noise, angular sampling and the number of observations. It is therefore a direct indication of the quality of any particular set of reflectance observations used to generate a retrieved albedo value. This can be compared with the constrained model inversion discussed in appendix 1, based on specifying that reflectance and directional hemispherical reflectance should lie between physically realistic limits (0 to 1).
6.6 Implications of negative model parameters

The negative values of the isotropic and volumetric model parameters seen in the 24th June barley and 23rd April wheat canopies raises the issue of what such negative model parameters mean and how they arise. In a physical sense a negative model parameter is meaningless: there cannot be negative volumetric or GO scattering, or by extension (and from energy conservation), negative reflectance. It is clear from these results however, and from other work (Disney et al., 1997; Hobson et al., 1999; Grant, 2000) that negative parameters can and do occur in practice. They arise as a result of the inversion process, with one parameter over-compensating for another in a case where reflectance is poorly described by the chosen kernel combinations. This implies that the correct choice of kernels may determine whether model parameters obtained through inversion have any physical meaning.

Practically, a better fit to measured reflectance data is generally obtained by allowing parameters to go out of physical bounds (i.e. to go negative) in order to compensate for the inability of the kernel combination to describe the shape of ρ_canopy. One or more parameters being out of physical bounds indicates that the kernel combination is fundamentally unable to describe the surface reflectance. Different approaches can be applied to this problem depending on the use to which the parameters are to be put. Negative model parameters may mean there is simply not enough information in the reflectance signal to provide an unequivocal solution to model inversion. In this situation, known as overfitting (Gershenfeld, 1999) the model has too much flexibility (too many free parameters) and can fit the data in a way that will not provide a physically meaningful solution. If inverted model parameters are to be interpreted directly e.g. for deriving LAI or crown density say, it may be appropriate to reduce the number of kernels (and hence model parameters) in order to reduce the number of degrees of freedom of the inversion and recalculate the parameter values. This was carried out for two of the canopies in figures 6.3 and 6.4 for which negative model parameters were obtained from the full linear model inversions (24th June barley and 23rd April wheat). Scatter plots showing the comparisons of the isotropic, volumetric and GO parameters, obtained from inverting two kernels with the corresponding parameters obtained from the three inverting kernels are presented in figures 6.6 and 6.7.
The scatter plots of figures 6.6 and 6.7 are laid out as follows:

Figure 6.6a (24th June barley canopy)
- isotropic (isotropic + RossThick) v isotropic (isotropic + RossThick + LiSparse)
- isotropic (isotropic + RossThin) v isotropic (isotropic + RossThin + LiDense)
- isotropic (isotropic + LiSparse) v isotropic (isotropic + RossThick + LiSparse)
- isotropic (isotropic + LiDense) v isotropic (isotropic + RossThin + LiDense)

Figure 6.6b (24th June barley canopy)
- volumetric (isotropic + RossThick) v volumetric (isotropic + RossThick + LiSparse)
- volumetric (isotropic + RossThin) v volumetric (isotropic + RossThin + LiDense)
- GO (isotropic + LiSparse) v GO (isotropic + RossThick + LiSparse)
- GO (isotropic + LiDense) v GO (isotropic + RossThin + LiDense)

Figure 6.7a (23rd April wheat canopy)
- isotropic (isotropic + RossThick) v isotropic (isotropic + RossThick + LiSparse)
- isotropic (isotropic + RossThin) v isotropic (isotropic + RossThin + LiDense)
- isotropic (isotropic + LiSparse) v isotropic (isotropic + RossThick + LiSparse)
- isotropic (isotropic + LiDense) v isotropic (isotropic + RossThin + LiDense)

Figure 6.7b (23rd April wheat canopy)
- volumetric (isotropic + RossThick) v volumetric (isotropic + RossThick + LiSparse)
- volumetric (isotropic + RossThin) v volumetric (isotropic + RossThin + LiDense)
- GO (isotropic + LiSparse) v GO (isotropic + RossThick + LiSparse)
- GO (isotropic + LiDense) v GO (isotropic + RossThin + LiDense)
a) 2 kernel v 3 kernel isotropic parameters.

b) 2 kernel v 3 kernel volumetric and GO parameters.

**Figure 6.6** Comparison of model parameters from 2 and 3 kernel inversions, 24th June barley.
Figure 6.7 Comparison of model parameters from 2 and 3 kernel inversions, 23rd April barley.
6.6.1 Discussion of two parameter inversions

Results presented in figures 6.6a and 6.7a show that where two kernels are inverted (isotropic and either \(k_{\text{vol}}\) or \(k_{\text{GO}}\)), the correlation with their three kernel counterparts is generally high in all cases, as would be expected. The differences are mostly ones of magnitude. The two kernel isotropic parameter is generally smaller than the three kernel version. The only exception to this is the isotropic parameter of the 24\textsuperscript{th} June barley canopy (figure 6.6a) derived from inversion of the isotropic + LiSparse kernel combination, which is slightly higher than the three kernel (isotropic + RossThick + LiSparse) isotropic parameter. Conversely, the volumetric and GO parameters from two kernel inversions are generally larger than their three kernel counterparts (figures 6.6b and 6.7b). In the case of the barley canopy the difference is only significant for the two kernel volumetric parameters. In this case the volumetric parameter obtained from inverting the isotropic + RossThick kernels is significantly larger than the three kernel volumetric parameter.

Most importantly, the volumetric parameter obtained from inverting the isotropic + RossThin kernels remains negative as it was in the original three kernel case (figure 6.4f). Neither the two kernel (isotropic + RossThin) nor the three kernel (isotropic + RossThin + LiDense) combinations are capable of describing reflectance behaviour and these kernels are clearly inappropriate for this canopy. The two kernel GO parameters are virtually identical to the three kernel versions suggesting that a combination of an isotropic and a GO kernel (either LiSparse or LiDense) is sufficient to describe reflectance for this canopy. Similar behaviour is apparent for the wheat canopy of 23\textsuperscript{rd} April (figure 6.7b). In this case, both the two kernel volumetric parameters are negatively correlated with their three kernel counterparts (almost perfectly in the case of the parameter derived from inversion of the isotropic + RossThin kernel combination), while the GO parameters are very similar to the three kernel versions.

These results indicate that in cases where inverted model parameters are negative, using two kernels as opposed to three is not likely to help. Two kernels are apparently sufficient to describe directional reflectance behaviour in some cases, particularly when appropriate choices of kernels are made (i.e. for these canopies, not the RossThin and/or LiDense kernels). Both the RMSE of model fit and the expected error in the derived
model parameters are higher in the inversion of the two kernel combinations than in the three kernel case. This is to be expected as the model has fewer degrees of freedom, and is unable to fit the measured reflectance so accurately. If the parameter values are to be directly interpreted however, the validity of the inverted parameters is of greater importance than the overall RMSE of model fit. If on the other hand the parameters are to be used indirectly e.g. for classification as mentioned previously, the requirement for physical constraint of model parameters is less clear. In this case the parameters are being used to provide only an indication of the relative spatial variation in scattering behaviour. Results presented above support this statement, suggesting that the relative magnitudes and spectral shapes of the inverted parameters are representative of the types of scattering occurring within the canopy even if their absolute magnitudes may be not be physically realistic (and should not be interpreted).

In the operational processing of reflectance data using linear models, the inversion process can be constrained to prevent negative parameters arising, via the use of Lagrange multipliers for example (see appendix 1). Constraints can also be imposed to ensure that products derived directly from model parameters such as directional-hemispherical and bihemispherical integrals of BRDF (so-called ‘black-sky’ and ‘white-sky’ albedos) lie within physically realisable limits i.e. between 0 and 1. Albedo values for given conditions of illumination and sky radiance can then be interpolated from these two limiting cases (Wanner et al., 1995). As discussed above, this type of approach is being taken for the processing of the EOS MODIS data products (Schaaf et al., 2000a,b; Gao et al., 2001; Schaaf et al., 2001a,b).

6.7 Conclusion

This chapter presents the results of experiments following on directly from those of chapter 4, which demonstrated that (with caveats) $\rho_{\text{canopy}}$ can be described as a linear combination of volumetric and GO scattering components. The experiments described in this chapter are designed to answer the second fundamental question regarding linear kernel-driven approach to modelling BRDF, namely whether the volumetric component of $\rho_{\text{canopy}}$ completely described by the volumetric kernel, and the GO component by the GO kernel i.e. are they separable? The simple answer is "No", but with provisos.
Understanding this issue is vital to determining the information it may be possible to retrieve by inversion of semi-empirical kernel-driven models against measured reflectance data.

Isotropic, volumetric and GO model parameters \((f_{iso}, f_{vol}, f_{GO})\) were derived from \(\rho_{canopy}\) in two distinct ways: i) via substitution of the parameters derived from regressing the volumetric and GO scattering components of (BPMS-simulated) \(\rho_{canopy}\) against \(k_{vol}\) and \(k_{GO}\) (a and b in tables 5.1, 5.2 and 5.3) into equations 6.2b and c, along with appropriate spectral estimates of \(\rho_{leaf}\) and \(\rho_{soil}\), and ii) via inversion of a full linear kernel-driven model against \(\rho_{canopy}\) calculated from substitution of the values of a and b (tables 5.1, 5.2 and 5.3) back into equation 6.1. This yielded spectral estimates of the angular model parameters. It was demonstrated that the volumetric and GO components of \(\rho_{canopy}\) are separable in some cases, with the volumetric parameter, \(f_{vol}\), closely approximating the shape of the chosen \(\rho_{leaf}\), and likewise \(f_{GO}\) and \(\rho_{soil}\). If the components were not separable, we would not expect \(f_{vol}\) and \(f_{GO}\) to resemble \(\rho_{leaf}\) and \(\rho_{soil}\) respectively, but would expect \(f_{iso}\), \(f_{vol}\) and \(f_{GO}\) to (equally) resemble some combination of them. This is apparent in some cases, where a significant proportion of the scattering from the canopy \((k_{vol})\) is taken up by the GO parameter, \(f_{GO}\). In all cases the isotropic parameter, \(f_{iso}\), showed some component of both \(f_{vol}\) and \(f_{GO}\), which is as expected. As the canopies developed the volumetric parameter came to more closely resemble the GO parameter implying that there is a degree of redundancy between the two kernels.

In order to examine the dimensionality of the separate components of \(\rho_{canopy}\) principal component analysis was performed on the volumetric and GO components. Results showed that the majority of the variance of each component was described by the corresponding kernel, as \(pc1\) in most cases was often greater than 80% and in many cases greater than 95% (mean value \(pc1\) was 81.6%). There was significant variation in the magnitude of \(pc1\) with \(\phi_{row}\). This implies that for certain canopies (e.g. those with relatively strongly row azimuth variation such as managed forest stands, or developing crops) there can be significant coupling of the kernels. This is another important fact in assessing the usefulness of parameter information derived from model inversion. The RossThick and LiSparse kernels are able to explain the most variance of the volumetric and GO components of \(\rho_{canopy}\) respectively. This supports the choice of the isotropic, RossThick LiSparse kernel combination as a model for use in general BRDF applications.
The occurrence of physically impossible (negative) model parameters arising from inversion was investigated. Such values typically occur when there are more degrees of freedom in the model than there are dimensions to the data (e.g. $\rho_{\text{canopy}}$ might only vary with in relation to two parameters, but three are used to try and describe it), or an inappropriate choice of kernels is used. In this case the model has too much freedom to fit the data and overfitting occurs. This is typical of an overdetermined system of more than $N$ equations in $N$ unknowns. Such a system can be very sensitive to small changes in the parameter values, particularly where measurement methods and approximations introduce noise into the parameter estimates (Twomey, 1996). This is the case for the inversion of semi-empirical BRDF models against measured reflectance data and the error inherent in inverted model parameters will be determined by the sampling strategy (Lucht and Lewis, 2000). The results presented here are all based on good angular sampling (in the solar principle plane, $\theta$, every $10^\circ$ and every $2^\circ$ around the hotspot). It is known that the linear kernel-driven models do not perform so well in cases where angular sampling is much poorer (Lucht and Lewis, 2000; Gao et al., 2001). It was shown that in some cases, two kernels can describe reflectance nearly as well as three kernels, but the choice of kernels becomes crucial in determining whether model parameters are negative. Where inverting three kernels resulted in strongly negative model parameters, using two kernels did not appear to give much better results. However, where three kernels results in parameters which are just negative, using two kernels can result in positive (and more physically realistic) model parameters.

If inverted model parameters are to be used indirectly, for example in spatial classification, then physically unrealistic parameter values are not necessarily a problem, as the kernels may still contain information related to (spectral and directional) scattering behaviour, although this is not the case if overfitting occurs. If the parameters are to be used directly however, then the inversion should be reduced to a constrained model parameter space. In this case, a combination of an isotropic term (there will always be a “brightness” component of surface reflectance) and either volumetric or GO kernels with parameter values constrained to lie within physically realisable limits, will prove a better solution. The choice of kernel becomes important in this case and for the barley and wheat canopies, the RossThick volumetric and LiSparse GO kernels appeared to work much better, either separately (in combination with the isotropic kernel) or as a three kernel combination.
It has been shown that although the inverted model parameters contain
biophysical information, it is likely to be coupled to a greater or lesser extent. Indeed,
spectral estimates of the angular model parameters show the influence of $\rho_{leaf}$ on the
inverted parameter estimates. This characteristic reflectance shape is common to all types
of green vegetation in the same way that BRDF shapes for certain surfaces have
significant commonality. The next chapter explores the idea that it may be possible to
develop a spectral analogue of the angular kernels in order to model spectral variations of
observed reflectance. This would have particular use for interpolating and extrapolating
limited spectral reflectance samples and could augment the angular kernels to provide a
full spectral, directional kernel-driven model of $\rho_{canopy}$. 
7 Development and application of spectral kernels

7.1 Introduction

The previous chapters have explored the detailed operation of the angular kernels in describing angular variations of canopy reflectance. Despite their approximate nature it is clear that they can be very successful in describing BRDF. The caveat is that care is required in order to interpret biophysical information contained in the model parameters. Importantly, the end result of providing a viable, working description of BRDF is promoted at the expense of physical accuracy (given the severely approximations nature the semi-empirical kernels). One reason for this is that the kernels were primarily designed with their integrated properties in mind, particularly for production of broadband albedo at moderate spatial resolutions, rather than for parameter retrieval and interpretation. They are intended merely to act as angular interpolants for limited samples of directional reflectance. As a result, the angular kernels take no account of spectral reflectance behaviour – they are independent of wavelength. Consequently, the analyses presented in chapters 4, 5 and 6 were expressly undertaken to be independent of wavelength. Despite this, it was shown that the angular kernels are sensitive to spectral variations in reflectance behaviour.

Accurate estimates of albedo are required in order to characterise the shortwave energy fluxes at the Earth’s surface, in particular for climate modelling. Land surface albedo is a measure of the proportion of incoming solar radiation reflected at the surface, and, more importantly, the quantity absorbed. As a result broadband albedo - across the spectral range of incoming solar radiation - is a lower boundary condition in models of global climate. However, albedo is generally parameterised in some way to overcome issues of measurement and spatial variability (Pinty et al., 2000; Strugnell et al., 2000). Henderson-Sellers and Wilson (1983) suggested that albedo is required to an accuracy of ±5% in order to be useful for climate studies. Sellers (1993) has since proposed a standard of accuracy in albedo measurements of ±2%. Given these constraints, the general insensitivity of the angular kernels to spectral variation, and the resulting limitation to production of narrowband estimates of albedo is clear. More than 40% of the total incoming solar energy lies in the visible to mid-IR region of the spectrum (0.35 and 0.7μm). In order to effectively describe surface energy fluxes, accurate estimates of albedo are required across this shortwave region (Justice et al., 1998). Conversion of limited spectral samples of albedo to a single broadband value requires a number of
assumptions and approximations. As outlined in section 2.1.1, spectral albedo can be convolved with the solar spectrum (Brest and Goward, 1987). In this case, albedo, $\alpha$, is calculated as

$$\alpha = \int_{\text{solar spectrum}} p(\lambda) \alpha(\lambda) d\lambda$$

where $p(\lambda)$ is the proportion of the total downwelling solar radiation at wavelength $\lambda$ (dependent on current atmospheric state); and $\alpha(\lambda)$ is spectral albedo, derived from the integration (with respect to the viewing and illumination geometry, $\Omega$ and $\Omega'$) of the angular kernels. These integrated terms provide estimates of (spectral) directional hemispherical and bihemispherical reflectance ($\hat{\rho}(\lambda, \Omega')$ and $\bar{\rho}(\lambda)$ respectively). $\alpha(\lambda)$ is then a weighted sum of these two components, with the weights determined by the relative quantities of direct and diffuse illumination. A drawback of this method is that it relies on being able to characterise the current atmospheric state, and success or failure in this respect will largely determine the accuracy of the results (Lewis et al., 1999). Liang et al. (1999, 2000) and Liang (2000) have shown that it is possible to use a series of pre-calculated conversion factors to calculate 'inherent surface albedo' (as opposed to 'apparent surface albedo' observed in the presence of atmospheric scattering) from narrowband measurements of reflectance. This method works quite well for calculating visible albedo, but less so for total shortwave albedo (Liang, 2000). In addition, radiative transfer simulations of atmospheric scattering are required to decouple surface and atmospheric components of TOA reflectance, which in turn rely on assumptions about atmospheric state, and/or the use of standard models of atmospheric scattering. Another approach is to use hyperspectral measurements of reflectance as a first pass at a spectral interpolant. Lucht et al. (2000) employed an observed hyperspectral reflectance profile as a spectral interpolant to convert spectral samples of satellite-observed albedo to broadband albedo (305-2800nm), rather than use an arbitrary spline curve. There is also a large body of work on spectral unmixing which seeks to extract (sub-pixel) areal proportions of so-called spectral end-members ('pure' vegetation and soil spectra) from multispectral reflectance measurements (Settle and Drake, 1993; van Leeuwen et al., 1997; Bateson et al., 2000).

This chapter presents a method of directly exploiting existing knowledge of variations in the **spectral** reflectance behaviour of soil and vegetation in order to interpolate limited samples of spectral canopy reflectance, $\rho_{\text{canopy}}(\lambda)$, over a much wider...
range of wavelengths (in particular 450-2500nm). In a direct analogy with the development of the angular kernels, it is proposed that $\rho_{\text{canopy}}(\lambda)$ can be split into constituent components of spectral soil and vegetation spectral reflectance, ($\rho_{\text{soil}}(\lambda)$ and $\rho_{\text{veg}}(\lambda)$) (c.f. separation of the volumetric and GO components of $\rho_{\text{canopy}}(\Omega, \Omega')$). Further, it is demonstrated that a small number of simple $\rho_{\text{soil}}(\lambda)$ and $\rho_{\text{veg}}(\lambda)$ terms can be combined in a weighted linear summation to describe the majority of observed variance in the behaviour of $\rho_{\text{canopy}}(\lambda)$. It will be shown that such terms (subsequently referred to as spectral kernels) can be readily derived and applied. More usefully, these spectral kernels can potentially be coupled with the angular kernels in order to provide a linear kernel-driven description of spectral directional canopy reflectance, $\rho_{\text{canopy}}(\lambda, \Omega, \Omega')$.

There are several key areas where such a development is likely to prove extremely useful:

i. **Generation of broadband albedo (across the visible, SWIR and NIR regions) from a potentially small number of narrowband samples.** As described above this is currently problematic as it is reliant on an ability to accurately characterise the atmospheric conditions under which reflectance measurements are obtained. The ability to interpolate limited spectral samples across the observed spectrum (essentially a spectral integral of $\rho_{\text{canopy}}(\lambda)$) is analogous to the use of the angular kernels to derive angular integrals of directional reflectance samples in order to derive $\bar{\rho}(\lambda, \Omega')$ and $\bar{\rho}(\lambda)$ (so-called black-sky and white-sky albedo).

ii. **Separation of the soil and vegetation scattering components of $\rho_{\text{canopy}}(\lambda)$.** This is of particular use for studies of radiation interception and photosynthetic efficiency. Parameters such as fAPAR are directly related to absorption of the photosynthetically active part of incoming solar radiation by vegetation within the canopy. The ability to isolate the spectral component of scattering originating from the vegetation would clearly be of benefit to such studies. The separation of the soil and vegetation components of $\rho_{\text{canopy}}(\lambda)$ is analogous to the separation of the volumetric and GO components of $\rho_{\text{canopy}}(\Omega, \Omega')$.

iii. **Making better use of limited directional/spectral sampling to improve BRDF model inversion.** The spectral kernels have the potential for exploring the meaning of derived spectral model parameters in the same manner as has been achieved with the directional kernels. This would permit better understanding of the impact of
spectral sampling on the accuracy of BRDF retrievals, similar to the way in which angular sampling has been explored (Lucht and Lewis, 2000).

iv. **Permitting the combination of multispectral data from sensors with different spectral bands and band-pass functions.** This would have the benefit of maximising the information extraction from of sensors with complementary spectral, spatial and temporal capabilities e.g. Meteosat Second Generation (MSG) (www[7.1]) and POLDER (www[7.2]). ‘Data synergy’ has long been an aim of remote sensing studies. Spectral kernels could be used to ‘normalise’ samples of spectral reflectance to a common set of wavebands. This is analogous to the use of angular kernels to normalise samples of directional reflectance obtained under arbitrary viewing and illumination conditions to a common viewing and illumination geometry (usually nadir).

### 7.2 Concept of spectral kernels

What is proposed is a series of simple functions that can be superposed in a weighted linear combination to describe the dominant shortwave (visible and NIR) reflectance characteristics of spectral canopy reflectance. This assumes that $\rho_{\text{canopy}}(\lambda)$ can be considered as follows

$$\rho_{\text{canopy}}(\lambda) = a_1 \rho_s + a_2 \rho_v + \left( a_3 \rho_s^2 \rho_v + a_4 \rho_s \rho_v^2 + a_5 \rho_v^3 + a_6 \rho_s^2 \rho_v^2 + \ldots \right)$$

where $a_i$ are constants; $\rho_s$ and $\rho_v$ are the single scattering contributions to $\rho_{\text{canopy}}$ from the soil and vegetation (reflectance or transmittance); terms in brackets are multiple scattering contributions representing higher order interactions between soil and vegetation (truncated). It should be recalled that the single scattered component of directional reflectance is the dominant feature, with successively higher orders of multiple scattering interactions becoming increasingly isotropic. The work of Price (1990) for soil, and Price (1992) and Hurcom *et al.* (1996) for vegetation suggest this is a reasonable assumption for $\rho_{\text{canopy}}(\lambda)$. Figure 7.1 demonstrates the dominance of the single scattered component of $\rho_{\text{canopy}}(\lambda)$ (note that the plot is logarithmic with respect to the reflectance...
Figure 7.1 Direct and diffuse scattering contributions to simulated $\rho_{\text{canopy}}$ as a function of scattering order (barley canopy, 15th May, nadir viewing and illumination).

contributions). In this example, the single scattered components contain 98% and 95% of the total contribution to reflectance in the direct and diffuse cases respectively (this is low, and is a result of the relatively sparse canopy).

If $\rho_{\text{canopy}}(\lambda) = (\rho_1, \rho_2, \ldots, \rho_n)$ is an observed reflectance spectrum for the set of $n$ wavelength values $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ then the desired spectral kernels (referred to by Price (1990) as basis functions) are $k(\lambda_1, \lambda_2, \ldots, \lambda_n)$, and

$$
\rho_{\text{canopy}}(\lambda) = \sum_{i=1}^{M} f_i k_i(\lambda)
$$

where the $f_i$ are the weights associated with each spectral kernel. The total number of basis functions, $M$, clearly cannot exceed the number of available bands, $n$, in the observed data (e.g. four in the case of MISR, and typically seven for MODIS), and ideally, $M \ll n$. This must suffice for a description of both the soil and vegetation components of $\rho_{\text{canopy}}(\lambda)$.

If such spectral kernels are plausible, they could be combined with the angular
kernels to create a spectral directional kernel-driven model of canopy reflectance. This situation is described in equation 7.4.

\[ \rho_{\text{canopy}}(\lambda, \Omega, \Omega') = [\rho_{\text{veg}}(\lambda) + \rho_{\text{soil}}(\lambda)] + [\rho_{\text{VOL}}(\Omega, \Omega') + \rho_{\text{GO}}(\Omega, \Omega')] \]

The spectral kernels would then provide a link between the spectral and directional domains, which is currently missing in the kernel-driven approach to modelling \( \rho_{\text{canopy}} \). The full spectral directional kernel-driven approach is then of the form

\[ \rho_{\text{canopy}}(\lambda, (\Omega, \Omega')) = \sum_{i=1}^{M} f_i k_i(\lambda) + \sum_{j=1}^{N} f_j k_j(\Omega, \Omega') \]

where \( N \) is the number of angular reflectance samples, and \( k_i \) and \( k_j \) are the spectral and directional kernels respectively. This approach considers the spectral and directional components of \( \rho_{\text{canopy}} \) as separate, and models each of them correspondingly as a linear sum of terms (kernels).

The remainder of this chapter presents a derivation of spectral kernels for \( \rho_{\text{soil}}(\lambda) \) and \( \rho_{\text{veg}}(\lambda) \) and demonstrates their use, in combination with the angular kernels, in describing modelled and observed spectral directional \( \rho_{\text{canopy}} \). The structure is as follows:

i) Derivation of spectral kernels from laboratory reflectance spectra, in particular \( \rho_{\text{veg}}(\lambda) \).

ii) Demonstration of kernels' ability to describe \( \rho_{\text{soil}}(\lambda) \) and \( \rho_{\text{veg}}(\lambda) \) individually, and \( \rho_{\text{canopy}}(\lambda) \).

iii) Demonstration of ability of spectral and directional kernels to describe \( \rho_{\text{canopy}}(\lambda, (\Omega, \Omega')) \).

iv) Discussion of implications, particularly in relation to the calculation of spectrally integrated products such as albedo.
7.3 Derivation of spectral kernels

The kernel-driven models of BRDF arose from the observation that it is possible to consider $\rho_{\text{canopy}}(\Omega, \Omega')$ as a sum of separate volumetric and GO terms (Roujean et al., 1992; Wanner et al., 1995). This approach considers $\rho_{\text{canopy}}(\Omega, \Omega')$ to be a sum of the dominant volumetric and GO "shapes" governing reflectance behaviour. The derivation of the angular kernels was described in detail in chapter 2, and the separability and information content of the two components was explored in chapters 4 and 5. The spectral kernels outlined below are derived from a similar observation: that $\rho_{\text{canopy}}(\lambda)$ can be considered as a combination of the spectral reflectance behaviour of soil and vegetation respectively. This work is based on that of several authors, notably Price (1990, 1992, 1998), who have noted that the major variations in reflectance behaviour of both soil and vegetation can largely be described by a few simple basis functions (spectral kernels).

7.3.1 Reflectance features of vegetation

It is well known that both vegetation and soil exhibit characteristic reflectance features (Carlson et al., 1971; Huete, 1989; Jacquemoud and Baret, 1990; Price, 1990; Curran et al., 1992; Asner, 1998). Different types of vegetation tend to differ far more in the relative magnitude of characteristic reflectance features than the wavelengths at which these features occur. Examples of leaf and soil spectra in figures 7.2 and 7.3 illustrate this.
Figure 7.2 Laboratory-measured vegetation reflectance spectra (Hosgood et al., 1994).

Figure 7.3 Field-measured soil and vegetation reflectance spectra (Milton, pers. comm.).
Figures 7.2 and 7.3 show both laboratory- and field-measured reflectance spectra of a variety of vegetation. Figure 7.3 contains spectra of a single leaf, a layered leaf medium, an optically thick leaf stack, and a pastille of powdered green leaf material. These spectra represent an extremely wide range of physical conditions (some artificial), yet the characteristic leaf reflectance features are present in all cases: the reflectance peak in the visible green (~550nm) due to chlorophyll pigments; the sharp rise in reflectance from the visible red to the shortwave IR (the so-called red-edge); water absorption features in the NIR at around 1450 and 1900nm. The spectra in figure 7.3 also display these similarities, albeit with wider variation due to external factors present in field measurements (atmospheric conditions, field of view considerations etc.). The difference between the soil spectra (in the visible at any rate) is essentially a linear transformation of scene brightness caused by the presence or absence of direct sunlight. The question remains as to whether the variation in the soil and/or the vegetation reflectance can be represented using simple terms in linear combination.

7.3.2 Soil kernels: the soil component of $\rho_{canopy}(\lambda)$

Price (1990) showed that the soil component of $\rho_{canopy}(\lambda)$ can be well-represented by a linear combination of basis functions, or kernels derived from measured spectra. Price (ibid.) applied principal component analysis (PCA) to laboratory-measured soil spectra of a wide range of soil types. PCA allows a set of correlated observations to be transformed to a set of uncorrelated (principal) components, or basis functions, by calculating the eigenvectors and eigenvalues of the variance-covariance matrix of observations. The percent variance in the data described by each PC is simply the corresponding eigenvalue, scaled by the sum of all eigenvalues (and multiplied by 100). The first PC describes the largest variance within the data, with subsequent PCs describing successively less of the observed variance. PCA permits the decomposition of observed spectra into PCs (spectral basis functions) which can then be summed to regenerate the original reflectance spectra.

Price (ibid.) showed that the first four PCs of laboratory-measured soil reflectance explained nearly 98% of the observed variance in the data, with the remaining variance attributable to measurement noise. Price's first four soil basis functions are shown in figure 7.4 (the functions are scaled in this case - the first basis function described over
Huete (1986) used factor analysis (closely related to PCA) to separate soil and vegetation spectral mixtures, whilst Huete and Escadafal (1991) applied spectral decomposition techniques (also closely related to PCA) to field-measured soil spectra. They found that four basis functions were sufficient to reconstruct observed spectra. Given the success of the spectral decomposition/PCA analysis of soil reflectance, and the use of Price's basis functions by a number of other researchers, notably by Nilson and Kuusk (1989) to describe $\rho_{soil}(\lambda)$ in their physically-based canopy reflectance model, it makes sense to use these basis functions as the soil spectral kernels in the spectral kernel-driven model of $\rho_{canopy}(\lambda)$. It then remains to derive corresponding vegetation kernels.

![Figure 7.4 Price's first four basis functions of observed soil reflectance spectra.](image)

It is apparent from figure 7.4 why Price's first basis function describes so large a proportion of the observed variance of soil reflectance. The rise across the visible and NIR parts of the spectrum is characteristic of soil reflectance, as are the water absorption features at around 1300 and 1900nm. The second and higher basis functions can act to moderate the first basis function depending on the visible and NIR reflectance behaviour of the soil being modelled.
7.3.3 Vegetation kernels: the vegetation component of $\rho_{canopy}(\lambda)$

The fact that spectral reflectance of vegetation has certain common features has been exploited by a number of researchers. Price (1992) showed that high resolution crop reflectance spectra measured in the field could largely be described using a weighted linear summation of the first five PCs of the observed data. Hurcom et al. (1996) used spectral decomposition to demonstrate that four factors (closely related to PCs) described 99.86% of observed spectral variance of semi-arid Mediterranean vegetation species. Some of these factors appeared to be correlated with biophysical properties such as the proportion of directly irradiated green leaf area viewed by the measurement instrument, and spectral response in the chlorophyll absorption region. Hurcom et al. (ibid.), and Hurcom and Harrison (1998), have also suggested that these vegetation factors could be used to describe the variation of spectrally similar vegetation types in terms of biophysical properties, rather than as mixtures of various spectral classes as in the standard mixture modelling approach. Indeed, work by Jacquemoud and Baret (1990), Baret et al. (1994) and Jacquemoud et al. (1996) has demonstrated that leaf reflectance is mainly controlled by a small number of physical parameters affecting leaf absorption behaviour (as opposed to scattering behaviour), such as leaf mesophyll structure, pigment concentration (chlorophyll a and b), and water, lignin and cellulose content. These are the minimum terms required to model leaf reflectance accurately. However, these terms are non-linear and so cannot be combined in a linear fashion as required here.

Following the approach of Price (1990, 1992), and Hurcom et al. (1996), vegetation spectral reflectance kernels (basis functions) have been derived through PCA of a large number of measured reflectance spectra. The primary difference between the analysis described here and Price’s work is the availability of both transmittance and reflectance spectra. This potentially permits the derivation of single scattering albedo kernels, given that single scattered albedo $\omega = \rho + \tau$. One of the aims of developing a linear kernel-driven model of $\rho_{canopy}$ is to allow broadband estimates of albedo to be derived from limited spectral samples. The most logical way to achieve this (and the most consistent with respect to energy conservation) is to use single scattering albedo from the outset.

Other differences from the analysis of Price (1990, 1992) are that the spectra used here were measured under laboratory conditions, rather than in the field where
measurement error increases due to atmospheric effects. In addition, the number and variety of spectra used are much greater, with nearly two thousand vegetation spectra, from one hundred and twenty distinct vegetation types. This compares with less than two hundred spectra of at most five crop types in Price's analysis. Finally, due to advances in computational capability it is now straightforward to carry out robust and accurate numerical inversions of matrices of the order of 2000 x 2000 in a few minutes. Price was forced to use numerical approximations in order to carry out piecewise inversions of significantly smaller matrices.

The reflectance and transmittance data used in this analysis were measured in the controlled environment of the European Goniometric Observatory (EGO) facility, at the Joint Research Centre (JRC), Ispra, Italy. These data were the result of the Leaf Optical Properties Experiment (LOPEX) (Hosgood et al., 1994), and formed the basis of work relating biochemical properties to reflectance (Jacquemoud et al., 1995) as well as for development of the PROSPECT-REDUX leaf reflectance model (Jacquemoud et al., 1996). A range of optical configurations are included within the LOPEX data, such as optically thick media (bark), fresh and dry (oven-dried) leaf samples, in addition to pastilles of powdered leaf samples, and fresh and dry leaf stacks (layered media) which are included to represent leaf-scale multiple scattering. It is known that the reflectance of oven-dried leaf spectra is not quite the same as naturally dry, brown vegetation and this will affect results slightly, in particular in the transition from visible to NIR wavelengths. However, it is intended that if/when naturally dry leaf spectra become available, these will be added to the analysis presented below. The spectra in figure 7.2 are drawn from the LOPEX data. Figures 7.5a and b show the (normalised) spectral vegetation kernels derived from the fresh and dry single scattered spectral albedo. These kernels are likely to be the most widely applicable, as they are derived from fresh and dry reflectance and transmittance spectra, as well as the pastille and leaf stack spectra. The latter spectra will potentially allow the kernels to describe at least the first order (spectral) multiple scattering terms of equation 7.2.

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1 Kindly provided by B. Hosgood, technical director of the EGO facility.
**Figure 7.5a** First five vegetation spectral kernels derived from fresh and dry single scattered albedo (450-1000nm).

**Figure 7.5b** First five vegetation spectral kernels derived from fresh and dry single scattered albedo (1000-2500nm).
The cumulative variance of the original data explained by each of the spectral kernels is given in table 7.1. The first and second kernels explain 83.9% and 14.5% of the observed variance respectively. The third component explains less than 1% of observed variance. This suggest that in most cases, two to three vegetation kernels should be sufficient to describe the majority of observed variance, particularly in the case of green vegetation. More kernels can be used (at the expense of requiring more spectral samples), but this will generally only serve to significantly improve fitting when the spectra diverge from healthy vegetation.

Table 7.1 First five eigenvalues of PCA of LOPEX fresh and dry single scattering albedo, and the corresponding percent variance.

<table>
<thead>
<tr>
<th>PC</th>
<th>eigenvalue</th>
<th>cumulative variance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>43.85</td>
<td>83.85</td>
</tr>
<tr>
<td>2</td>
<td>7.56</td>
<td>98.31</td>
</tr>
<tr>
<td>3</td>
<td>0.39</td>
<td>99.05</td>
</tr>
<tr>
<td>4</td>
<td>0.11</td>
<td>99.50</td>
</tr>
<tr>
<td>5</td>
<td>0.067</td>
<td>99.71</td>
</tr>
</tbody>
</table>

The reduction in explained variance from PC 1 to 2 in this case is smaller than for any of the other possible combinations of LOPEX spectra. For example, if only fresh leaf reflectance is used, the first PC explains 95.8% of observed variance, and the second, 3.4%. If dry leaf transmittance is used, the first PC explains 96.5% of observed variance, and the second PC, 2%. As a result, these combinations are likely to permit fewer vegetation kernels to be used to model a given set of observations of $\rho_{\text{canopy}}(\lambda)$. However, the ability to describe albedo directly is of greater importance, and hence the combination of fresh and dry single-scattered albedo is thought the most appropriate at this stage.
7.4 Testing the spectral kernels

The first step in demonstrating the applicability of the spectral kernels is to show they can reconstruct independently measured soil and vegetation spectra. These data are provided by the Natural Environment Research Council Equipment Pool for Field Spectroscopy (NERC EPFS), based at Southampton University, from spectra measured in a variety of locations and (field) conditions. The EPFS data comprise 85 spectra of various cover types (not just soil and vegetation), measured using a 15° FOV hand-held radiometer, with a wavelength range of 400 to 1000nm in steps of 1nm. Results are presented from inversions of spectral kernels derived from fresh and dry leaf reflectance and transmittance as well as fresh and dry single scattered albedo, against all available observed spectra. This is to examine the limitations (if any) of using only the fresh and dry single scattered albedo spectral kernels to reconstruct observed spectra. Following this, specific examples of inversions of the derived spectral kernels against field-measured reflectance are presented, such as green and senescent vegetation. Following this, results are presented for inversion of both spectral and directional kernels simultaneously against spectral, directional reflectance samples generated using a physically-based (radiative transfer) model of canopy reflectance (the model of Nilson and Kuusk, 1989). In this case, samples of reflectance are simulated with θ, varying from -75 to 75 degrees (θ, = Φ, = 0°) in steps of 5°, with spectral bands from 400 to 2500nm in steps of 20nm. This is designed to test the kernels' ability to fit the spectral component of ρcanopy, related to ρleaf. Although ρcanopy contains a significant (non-linear) multiple scattering component, a linear combination of kernels (including a kernel related to multiple scattering, derived from leaf stack spectra) may be capable of describing spectral variation in this case. Lastly, the spectral kernels are inverted against multi-spectral ATM data (described in section 3.1.5).

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2 Many thanks to Dr. E. Milton and colleagues at EPFS for use of the field data.
7.4.1 Inversion against all NERC EPFS spectra

The results presented in figures 7.6, 7.7 and 7.8 illustrate the kernels' performance in inversion against the entire EPFS data, containing spectra of (amongst other things) concrete, water, gorse, limestone and vegetation. These surfaces cover a variety of spectra that are likely to be found in the pixels of a moderate (km-scale) resolution satellite image of the land surface.

Figure 7.6 Cumulative relative error of inversion of vegetation spectral kernels derived from fresh and dry reflectance and transmittance spectra, against all EPFS spectra.
Figure 7.7 Cumulative relative error of inversion of vegetation spectral kernels derived from fresh single scattering albedo only, against all EPFS spectra.

Figure 7.8 Cumulative relative error of inversion of vegetation spectral kernels derived from fresh and dry single scattering albedo, against all EPFS spectra.
Figures 7.6, 7.7 and 7.8 shows the cumulative (relative) error frequency for inversion of the kernels against all 83 spectra included in the EPFS data set. The vertical axis represents the percentage of samples in total with RMSE below this level and the horizontal axis shows the RMSE at that cumulative error level. There is a noticeable increase in RMSE at around the 90% cumulative relative frequency level (except for the five kernel case). This error level, at which 90% of inversions have a lower error, is used as a comparison between the various cases. The fresh and dry reflectance and transmittance (ρ and τ) case (figure 7.6) is included to examine whether using single scattering albedo confers any advantage over using reflectance or transmittance spectra alone. The ρ and τ cases are separable on RMSE at the 90% level, particularly in the one to three kernel cases. Results are presented in table 7.2.

Table 7.2 RMSE of inversion of various kernel combinations against field-measured spectra.

<table>
<thead>
<tr>
<th>no. of kernels</th>
<th>fresh + dry ρ</th>
<th>fresh + dry τ</th>
<th>fresh ω</th>
<th>fresh + dry ω</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.09</td>
<td>0.1</td>
<td>0.11</td>
<td>0.106</td>
</tr>
<tr>
<td>2</td>
<td>0.046</td>
<td>0.042</td>
<td>0.04</td>
<td>0.106</td>
</tr>
<tr>
<td>3</td>
<td>0.016</td>
<td>0.028</td>
<td>0.02</td>
<td>0.064</td>
</tr>
<tr>
<td>4</td>
<td>0.019</td>
<td>0.013</td>
<td>0.014</td>
<td>0.063</td>
</tr>
<tr>
<td>5</td>
<td>0.009</td>
<td>0.009</td>
<td>0.008</td>
<td>0.013</td>
</tr>
</tbody>
</table>

As might be expected, increasing the number of kernels improves the ability of the spectral kernels to recreate measured spectra. As might also be expected, increasing the number of kernels produces progressively less improvement each time. Kernels derived from reflectance or transmittance spectra alone exhibit broadly similar characteristics. For a fixed number of kernels those derived from fresh spectra tend to perform slightly better than the same number derived from dry spectra. Kernels derived from both fresh and dry reflectance spectra generally performed better than those derived from fresh and dry transmittance spectra. Operationally, it is preferable to keep the number of spectral kernels to an absolute minimum so that the number of bands required for inversion is kept small (ideally less than seven). Given that between two and four soil kernels will be required in order to describe the ρsoil(λ) component of ρcanopy(λ), it is desirable that the ρveg(λ) component of ρcanopy(λ) can be described by two or three vegetation kernels.

Figures 7.9a and b show the relative error of inversion (mean RMSE as a fraction of mean reflectance) for all the various EPFS field-measured reflectance spectra. RMSE
for the one and four kernel cases are shown for all samples. In the cases where the spectra resemble green vegetation spectra closely, the relative error is between 5% and 10%. The difference in error between using one or four kernels is small. As the spectra depart from green vegetation (asphalt, concrete, limestone and water), relative error increases and the difference between the one and four kernel cases becomes larger, doubling in the most extreme cases. This demonstrates further that two kernels may well be sufficient to describe reflectance of green vegetation. Figures 7.10a and b show spectral plots of measured and modelled lush and dry grass spectra in the visible and NIR respectively. Although there is excellent general agreement, it can be seen that differences tend to be concentrated in the visible part of the spectrum. This is not necessarily desirable for studies of albedo, as the incoming solar radiation is at a maximum here, which will tend to exacerbate such errors.

Figure 7.9a Relative error of inversion, EPFS reflectance spectra samples 1-47, 1 and 4 kernels.
Figure 7.9b Relative error of inversion, EPFS reflectance spectra samples 48-83, 1 and 4 kernels.
Figure 7.10a Original and modelled lush and dry grass spectra, 1 and 4 kernels, visible.

Figure 7.10b Original and modelled lush and dry grass spectra, 1 and 4 kernels, NIR.
7.4.2 Demonstration of vegetation spectral kernels against specific measured spectra

Figures 7.11a and b show scatter plots of measured against modelled reflectance of the lush grass and dry grass spectra shown in figure 7.10. These spectra representing a broad range of vegetation reflectance characteristics, from healthy, green vegetation to senescent. The spectra were measured in the field under varying atmospheric conditions, so providing a stern test of the kernels' flexibility. In each case, one to five vegetation kernels are used to derive the forward modelled reflectance spectra. Using more kernels is always more likely to provide a better fit to the observed data due to the increased degree of freedom (assuming overfitting is not occurring), at a cost of requiring more spectral bands.

![Figure 7.11a Measured against modelled lush grass reflectance, 1 - 5 vegetation kernels.](image)

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Figure 7.11b Measured against modelled dry grass reflectance, 1 - 5 vegetation kernels.

It can be seen from figure 7.11a that there is close correlation between the measured and modelled lush grass reflectance (r values greater than 0.98 in all cases). There is greater variation in the scatter of the dry grass reflectance values (figure 7.11b, r around 0.95), in particular at visible parts of the spectrum (lower values of reflectance). The pattern of variation in the RMSE is not unexpected. The lush grass has by far the lowest RMSE and, although the error reduces as the number of kernels increases, the reduction is relatively small (0.0099 for 1 kernel to 0.0065 for 5 kernels). This illustrates that when fitting spectra of green vegetation, only one or perhaps two kernels are necessary to achieve a good fit, simply because of the close resemblance of, in particular the first kernel, to the general green leaf reflectance shape. The RMSE in the case of dry grass is approximately double that of the lush grass case, with the exception of the five kernels case where the RMSE values are comparable (0.020 for 1 kernel, 0.0056 for 5 kernels). This demonstrates that a larger number of vegetation spectral kernels can, if necessary, fit a wide range of spectra. The addition of more kernels will allow more flexibility, but it is not necessarily desirable to allow the kernels to fit any kind of reflectance as they are intended in part to allow the separation of vegetation and soil spectra from \( \rho_{\text{soil}}(\lambda) \).
Figure 7.12 shows the residual error between the measured and modelled lush and dry grass reflectance values shown in figure 7.10. There are two main areas of difference - firstly in the visible green and red (500-650nm) where the modelled reflectance tends to be on the low side in the lush grass case, particularly in the regions of strong chlorophyll absorption at around 580nm. The one and four kernel cases are virtually identical. However, for the dry grass case they differ in the visible region, with the one kernel case over-estimating reflectance, while the four kernel case has a much smaller residual error. Across the red edge and into the NIR the lush grass case has a very low residual error, while the modelled dry grass reflectance overestimates the measured values. This is largely a function of the difference in the position of the red edge in the dry grass spectra. The gradient of the spectral reflectance at this point is such that if the red edge position is very slightly out, the differences between measured and modelled values will be amplified.

![Residual Error Graph]

**Figure 7.12** Residual error between measured and modelled lush and dry grass reflectance, one and four kernel cases.

It is worth noting that RMSE may not be the most appropriate measure of fitting error in the case of modelling vegetation spectra. There may be regions of close agreement between measured and modelled spectra in some parts of the spectrum and disagreement in others and RMSE over the whole spectrum will not reflect this. Other
error measures based on specific features of observed vegetation reflectance may be more instructive. For example, discrepancies in the red edge position between measured and modelled spectra may represent the ability of spectral kernels to reconstruct spectral reflectance in the visible and NIR more accurately than RMSE. Red edge position also has the advantage of being (empirically) related to the biophysical properties of vegetation (particularly in the visible and NIR).

Another measure of goodness of fit might be a spectral index such as NDVI (Normalised Difference Vegetation Index) (Rouse et al., 1974) which is simply the difference between the NIR and visible red signal divided by their sum. A more general measure of the suitability of a particular model (in this case represented by type and number of spectral kernels) is an information criterion (IC) such as that of Akaike (1974) (AIC). AIC balances the (log) maximum likelihood selection of a particular model against both the number of observations and the number of free model parameters. Table 7.3 shows the results of applying these three criteria to the inversions of one and five (fresh and dry single scattering albedo) spectral kernels against lush and dry grass spectra (Δ values represent differences from the original spectra; lower AIC values represent better model fit). The red edge position in table 7.3 is calculated by finding the wavelength at which $\frac{\partial^2 \rho}{\partial \lambda^2} = 0$. Red edge position in this case is defined as the wavelength (between 670 and 750nm) where the gradient of $\rho(\lambda)$ is at its steepest. At this point, the derivative of $\rho(\lambda)$ will be at a maximum, and hence the second derivative will be zero.

<table>
<thead>
<tr>
<th>Grass spectra</th>
<th>RMSE 1k</th>
<th>RMSE 5k</th>
<th>Δ(NDVI) 1k</th>
<th>Δ(NDVI) 5k</th>
<th>Δ(red edge)/nm 1k</th>
<th>Δ(red edge)/nm 5k</th>
<th>AIC 1k</th>
<th>AIC 5k</th>
</tr>
</thead>
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<tr>
<td>dry1</td>
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<td>0.019</td>
<td>0.089</td>
<td>0.021</td>
<td>5</td>
<td>2</td>
<td>-414.3</td>
<td>-646.6</td>
</tr>
<tr>
<td>dry2</td>
<td>0.042</td>
<td>0.019</td>
<td>0.098</td>
<td>0.015</td>
<td>5</td>
<td>2</td>
<td>-465.8</td>
<td>-630.0</td>
</tr>
<tr>
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<td>0.017</td>
<td>0.123</td>
<td>0.016</td>
<td>0</td>
<td>3</td>
<td>-433.9</td>
<td>-684.4</td>
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<tr>
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<td>0.015</td>
<td>0.195</td>
<td>0.015</td>
<td>6</td>
<td>2</td>
<td>-379.4</td>
<td>-699.6</td>
</tr>
<tr>
<td>lush1</td>
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<td>0.024</td>
<td>0.026</td>
<td>0.069</td>
<td>10</td>
<td>9</td>
<td>-587.2</td>
<td>-653.2</td>
</tr>
<tr>
<td>lush2</td>
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<td>0.027</td>
<td>0.019</td>
<td>0.089</td>
<td>14</td>
<td>10</td>
<td>-549.7</td>
<td>-626.3</td>
</tr>
<tr>
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<td>0.027</td>
<td>0.001</td>
<td>0.084</td>
<td>14</td>
<td>9</td>
<td>-519.3</td>
<td>-633.1</td>
</tr>
<tr>
<td>lush4</td>
<td>0.028</td>
<td>0.024</td>
<td>0.012</td>
<td>0.067</td>
<td>11</td>
<td>9</td>
<td>-571.9</td>
<td>-648.1</td>
</tr>
<tr>
<td>lush5</td>
<td>0.048</td>
<td>0.033</td>
<td>0.018</td>
<td>0.097</td>
<td>14</td>
<td>9</td>
<td>-457.3</td>
<td>-583.9</td>
</tr>
</tbody>
</table>

In this case, the various measures exhibit broadly the same trends as RMSE (particularly AIC). However certain features are emphasized e.g. Δ(NDVI) varies more strongly then RMSE in the 1 kernel lush grass case and is actually more sensitive
generally. Table 7.3 highlights the fact that RMSE may not always be the best (or most appropriate) measure of model fit, particularly when modelling biophysical processes. This fact should be considered (along with parameter constraint and energy conservation requirements) in any implementation of a full spectral directional kernel-driven model of $\rho_{\text{canopy}}$.

7.5 A spectral directional kernel-driven model of $\rho_{\text{canopy}}$

In order to test the spectral kernels fully (as they would be applied in practice) they must be applied in conjunction with the angular kernels (equations 7.4 and 7.5) to samples of spectral directional reflectance. In order to provide a stable comparison (avoiding the ambiguities that may be introduced at all stages during field measurement of such data), spectral directional reflectance data were generated using the physically-based canopy reflectance model of Nilson and Kuusk (1989). This model was used as it can be run in forward and inverse modes quite rapidly. Reflectance data were generated for canopy configurations as follows:

- LAI of 0.1 and 4 (sparse and dense canopy cases).
- $\theta_i$ varying from -75 to 75 degrees ($\theta_i = \phi_{t,v} = 0^\circ$) in steps of 5°.
- Spectral bands varying from 400 to 2500nm in steps of 20nm.

![Figure 7.13 Simulated $\rho_{\text{canopy}}$, LAI = 0.1, $\theta_i = 0^\circ$](image)

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Figures 7.13 and 7.14 show the simulated spectral directional $\rho_{\text{canopy}}$ data for low and high LAI cases (0.1 and 4 respectively). The LAD for each canopy was uniform. Spectrally, the low LAI case is unsurprisingly very close in shape to soil reflectance, while the high LAI case is typically characteristic of vegetation. In directional terms, the low LAI canopy possesses a shallow, inverted 'bowl-shape' with a relatively low overall magnitude (maximum of around 30%). The high LAI case is relatively flat in the visible region, with a peak in the hotspot direction but is more significantly peaked across the red edge and into the NIR. Reflectance is generally higher overall in this case, rising to close to 70% at nadir in the NIR.

The full spectral directional linear kernel-driven model (equations 7.2 and 7.4) was inverted against the simulated $\rho_{\text{canopy}}$ data, generating modelled estimates of directional and spectral reflectance, each with the associated model kernel weights, forward modelled reflectance components, and RMSE values. The spectral kernels were inverted against the spectral estimates of $\rho_{\text{canopy}}$ (first term of equation 7.5) while the angular kernels were inverted separately against the angular samples of $\rho_{\text{canopy}}$ in each waveband (second term of equation 7.5). It should be noted that in future applications the set of kernels will include spectral and angular terms, which will be inverted together against $\rho_{\text{canopy}}$. In this way the kernels will be explicitly linked. This raises the possibility that the spectral kernels may end up fitting angular reflectance variations (and vice versa).
as the inversion process simply minimises $e^2$ between observed and modelled values of $\rho_{\text{canopy}}(\lambda, (\Omega, \Omega'))$, and does not discriminate between "angular" and "spectral" variation. However it is likely that the fit of spectral kernels to $\rho_{\text{canopy}}(\lambda)$ and angular kernels to $\rho_{\text{canopy}}(\Omega, \Omega')$ will achieve this. If necessary, constraints can be applied to enforce this.

As in previous chapters, the RossThick and LiSparseModis kernels are used (volumetric and GO kernels respectively). The spectral kernels are applied in varying combinations to modelling the spectral component of the simulated samples of $\rho_{\text{canopy}}$. The number of separate soil and vegetation spectral kernels applied to each set of simulated $\rho_{\text{canopy}}$ (varying LAI) is varied between one and three. Hence, the minimum total number of spectral kernels is two (one soil and one vegetation) and the maximum is six (three soil and three vegetation). Results are presented as follows:

- Original spectral reflectance against reflectance reconstructed using spectral kernels and scatter plots of one against the other.
- Analysis of RMSE and residuals for different numbers of kernels.
- Original directional reflectance against reflectance reconstructed using angular kernels and scatter plots of one against the other.
- Directional component of reconstructed spectral reflectance and comparison with spectral component of reconstructed directional reflectance (c.f. chapter 6).
7.5.1 Performance of spectral kernels against simulated spectral directional $\rho_{\text{canopy}}$

![Graph showing spectral reflectance for different LAI cases and kernel combinations.](image)

Figure 7.15 Demonstration of spectral kernels' ability to reconstruct spectral reflectance for two LAI cases, for two separate kernel combinations ($\theta_r = \theta_i = 0^\circ$).

Figure 7.15 shows results from inverting a spectral kernel-driven model against simulated $\rho_{\text{canopy}}$ (labelled original) for low and relatively high LAI canopies (0.1 and 4 respectively). Inversions of one soil plus one vegetation kernel (labelled s1v1), and three soil plus three vegetation kernels (labelled s3v3) are shown. It can be seen immediately that in most cases the spectral kernels do an excellent job of reconstructing $\rho_{\text{canopy}}(\lambda)$, particularly across the red edge in the high LAI case and in the NIR. An exception to this is for the low LAI canopy when only two kernels are used. This configuration lacks the flexibility required to accurately reconstruct observed reflectance. As a result the forward modelled reflectance spectra overestimate reflectance in the visible and SWIR and underestimate at longer wavelengths. This inflexibility is also apparent in the high LAI case, particularly in the water absorption features at 1600 and 1850nm where reflectance is over-estimated by the s1v1 kernel combination. RMSE values for these inversions are given in table 7.4. In terms of using a spectral kernel approach to derive albedo, the magnitude of RMSE suggests that more than one soil and vegetation kernel should be used, in order to keep error below 1 or 2% if possible.
Table 7.4 RMSE of inversion of spectral kernels against reflectance data.

<table>
<thead>
<tr>
<th>LAI</th>
<th>kernel combination</th>
<th>RMSE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>s1v1</td>
<td>3.96</td>
</tr>
<tr>
<td>0.1</td>
<td>s3v3</td>
<td>0.086</td>
</tr>
<tr>
<td>4</td>
<td>s1v1</td>
<td>3.67</td>
</tr>
<tr>
<td>4</td>
<td>s3v3</td>
<td>0.981</td>
</tr>
</tbody>
</table>

Figures 7.16 and 7.17 show scatter plots of original against forward modelled reflectance for the low and high LAI cases, for each kernel combination (s1v1, s2v3, s3v3) and for three separate view zenith angles (nadir, 30° and 60°). For the LAI = 0.1 case, correlation increases dramatically from the two to four kernel cases, less so for the four to six kernel cases. Again, the largest discrepancies appear at lower reflectance values, particularly for the s1v1 case. The LAI = 4 case shows distinctly higher correlation for the s1v1 cases. In the low LAI case, \( r^2 \) tends to decrease with decreasing view zenith angle, particularly for the s1v1 case. The reverse is true for the high LAI case.

Figure 7.18 shows a scatter plot of the combined results presented in figures 7.16 and 7.17. The correlation for both LAI cases is generally high, with the LAI = 4 having a slightly higher value of \( r^2 \). The disagreement is greatest at lower reflectance values (below 0.15) as observed previously. Figure 7.18 illustrates clearly the effectiveness with which the spectral kernels can model the spectral component of \( \rho_{canopy}(\lambda, (\Omega, \Omega')) \), particularly if more than one soil and vegetation kernel are used. Results illustrating the separation of the vegetation and soil component are shown in the next section.
Figure 7.16 Original against modelled reflectance, LAI = 0.1.

Figure 7.17 Original against modelled reflectance, LAI = 4.
Figure 7.18 Scatter plot of all view zenith angles and kernels combinations.

Figure 7.19 shows the residuals associated with the model fitting of figures 7.16 and 7.17. The residuals indicate that the model fit is (unsurprisingly) poorest for the two kernel case (s1v1) for both canopies. In particular, the kernels underestimate reflectance in the visible by up to 7% for both canopies. In the NIR, results differ for the two canopies, with the kernels continuing to underestimate reflectance in the LAI = 0.1 case, and overestimate in the LAI = 4 case. The residuals swap signs at around 1380nm before fluctuating in the 2000nm range as a result of the inability to follow the water absorption features. The residuals for the six kernel cases (s3v3) are very much smaller, indicative of the better fit obtained. The residuals in the case of the low LAI canopy are close to zero across the spectrum, while for the high LAI case, the only significant residuals are in the visible region, with residuals of around +/-3%.
7.5.2 Separation of soil and vegetation components

One aim of developing the spectral kernels is to allow the separation of the spectral soil and vegetation components of $\rho_{\text{canopy}}(\lambda)$. Results presented below show the spectral components of soil and vegetation reflectance extracted with the spectral kernels from the original $\rho_{\text{canopy}}$ values. Figures 7.20 and 7.21 show the original spectral reflectance, as well as the modelled soil and vegetation components for the low and high LAI canopies respectively. The components of the two and six kernel inversions are shown and labelled respectively as $s1, v1$ ($k=2$) and $s[1,2,3] v[1,2,3]$ ($k=6$), where the $s$ and $v$ represent the number of soil and vegetation kernels respectively, as before. If the kernels are able to separate the spectral soil and vegetation components of $\rho_{\text{canopy}}$, it would be expected that the soil kernels would dominate the soil component with minimal contribution from the vegetation kernels and the vegetation kernels would dominate the vegetation component.
Figure 7.20 Soil and vegetation model parameters, LAI = 0.1.

Figure 7.21 Soil and vegetation model parameters, LAI = 4.
For the low LAI canopy single case, the single soil parameter dominates reflectance as would be expected. However, the vegetation parameter is exclusively negative (acting to reduce overall reflectance) indicating that one soil kernel is not sufficient to describe the soil component accurately. The soil parameter strongly overestimates reflectance in the visible and SWIR but matches reflectance quite closely at longer wavelengths, particularly in the water absorption feature at 1850nm. For the six kernel case, the first two parameters dominate the modelled reflectance and the third soil parameter is very much smaller, suggesting that two soil kernels may well be enough in some cases. The vegetation parameters are all close to zero.

For the high LAI case, the separation of the soil and vegetation components is even clearer. In both the two and six kernel cases the vegetation parameters dominate reflectance. In the former case, although the single vegetation parameter dominates, particularly in the visible and NIR regions, the soil parameter contributes up to about 15% of total reflectance, mainly beyond 1000nm. For the six kernel case, the first vegetation parameter is significantly larger than the corresponding parameter in the two kernel case, with the first soil parameter being lower. The remaining two soil parameters are close to zero. These results indicate that the kernels are quite capable of separating soil and vegetation components of spectral reflectance, even in a potentially tricky case such as a high LAI canopy where the single scattering contribution to soil reflectance is likely to be small due to the density of the canopy.

Figures 7.22 and 7.23 are scatter plots of all soil and vegetation components of forward modelled reflectance respectively, for both LAI cases. Correlation for the soil component is almost identical for both canopies (r² values of 0.837 and 0.833 respectively). There is, however, a significant negative component for the high LAI canopy, where the magnitude of the original soil component is very low, and is generally much smaller than the vegetation component. However, the primary conclusion is that the soil kernels can successfully separate the soil component of ρ_canopy and do it equally well for high or low LAI canopies.

Correlation between the original and forward modelled vegetation components of the low LAI canopy shown in figure 7.23 is close to zero. This suggests that the vegetation kernels have trouble separating out the vegetation component of ρ_canopy when it is small in comparison to the soil component. For the high LAI case correlation is
virtually the same as in both the soil cases ($r^2$ value of 0.83). The modelled vegetation component is overestimated by around 7-10\% across all values. This is reflected in the slope of the regression relation (0.9) and the intercept of 0.09. These two results suggest the soil kernels are perhaps more flexible in being able to separate out the soil component in both high and low LAI canopies. The vegetation kernels can also separate out the vegetation component from $\rho_{\text{canopy}}$, but tend to struggle when the soil component dominates.

**Figure 7.22** Scatter plot of soil components of $\rho_{\text{canopy}}$, two LAI cases.
Figure 7.23 Scatter plot of vegetation components of \(\rho_{\text{canopy}}\), two LAI cases.

7.5.3 Reconstruction from limited wavebands

Reconstruction of full spectrum reflectance has so far been carried out by inverting kernels against reflectance samples generated at wavelength intervals of 20nm from 400 to 2500nm. In order to demonstrate the kernels' ability to interpolate from limited samples of reflectance, a brief demonstration of the inversion of the kernels against selected MODIS wavebands at visible and NIR wavelengths is presented. A limited set of available MODIS wavebands was selected to coincide with (in particular) visible blue, green and red, as well as NIR reflectance features. These bands are 443.0, 469.0, 555.0, 645.0, 858.5, and 940.0nm. The small number of bands provides a more stringent test of the kernels' ability to interpolate (and potentially extrapolate) limited reflectance samples and reconstruct full spectra. Figure 7.24 shows the inversion of the s1v1 and s3v3 kernel combinations against six reflectance bands.
Figure 7.24 Reflectance generated from samples at selected MODIS wavebands.

Figure 7.24 shows that the spectral kernels can reconstruct full spectrum reflectance from limited wavebands very effectively. Even with only six reflectance bands (just enough to perform a valid inversion) the forward modelled reflectance agrees extremely closely with the original values, particularly for the s3v3 case. The RMSE values in each case are correspondingly small, 9x10^{-3} for both s1v1 cases and 4x10^{-7} for the s3v3 cases. If the reconstructed spectra are to be used for spectral interpolation (e.g. for production of broadband shortwave albedo), rather than direct interpretation, then the spectral kernels may permit better use to be made of available reflectance information than is currently the case. Typically, broadband albedo is derived from limited samples using simple convolution across the solar spectrum, or with empirical coefficients derived for particular sensors (Liang, 2000; Liang et al., 2000c).

Figure 7.25 shows scatter plots of original against forward modelled reflectance values given in figure 7.24. The correlation is extremely high, with r^2 values exceeding 0.99 in all cases. It should be noted that in practice, spectral sampling will become an issue for the application of spectral kernels as angular sampling is for the angular kernels (Lucht and Lewis, 2000). The location of spectral samples (and the bandpass of the
instrument under consideration) will have an impact on the error associated with inversion of the spectral kernels against spectral reflectance data.

![Figure 7.25 Scatter of reflectance generated at selected MODIS wavebands (1 soil + 1 vegetation and 3 soil + 3 soil kernels).](image)

### 7.5.4 Directional component

Following analysis of the spectral kernels' ability to reconstruct the spectral component of $\rho_{canopy}(\lambda, \Omega, \Omega')$ the directional component of the spectral kernels is briefly examined. Although the spectral kernels are independent of view zenith angle (in the same way that the angular kernels are independent of wavelength), they may contain directional information. This is analogous to the spectral variation seen in the inverted directional kernels shown in chapter 6. Figure 7.26 shows the soil and vegetation spectral kernel parameter values for the s1v1 case plotted as a function of view zenith angle (the s3v3 cases are not shown as they follow the same patterns but with each successively reducing in magnitude). For the low LAI canopy the soil kernel, s1, dominates as expected. The angular variation of s1 is characteristic of the GO component of $\rho_{canopy}(\Omega, \Omega')$. 
\( \Omega' \) seen in chapter 4. The vegetation kernel, \( \mathbf{v}_1 \), is close to zero, as expected. For the high LAI canopy, the soil kernel is slightly above zero while the vegetation kernel is sharply peaked in the hotspot direction. This strongly resembles the directional variation of the volumetric component of \( \rho_{\text{canopy}}(\Omega, \Omega') \) seen in chapter 4.

![Angular variation of inverted spectral kernel parameter values (s1v1 case).](image)

**Figure 7.26** Angular variation of inverted spectral kernel parameter values (s1v1 case).

The observation that the soil and vegetation spectral kernels contain angular information related to the GO and volumetric angular kernels is confirmed by regression of the spectral kernel parameter values against the respective volumetric and GO components of BPMS simulated canopy reflectance. Using volumetric and GO components of BPMS-derived canopies with similar LAI to those used above (wheat canopy of 23\(^{\text{rd}}\) March, LAI = 0.9; barley canopy of 13\(^{\text{th}}\) May, LAI = 3.9) \( r^2 \) values of greater than 0.95 were obtained for the GO components of both canopies. Values of \( r^2 \) for the relationship between volumetric components were greater than 0.85. These results indicate that the spectral kernels are likely to contain angular information when inverted against directional data.

It is intended that the spectral kernels be developed more fully, integrated with the angular kernels into a spectral directional kernel-driven model and tested on airborne and spaceborne remote data, with the eventual aim of producing spatial estimates of spectral
7.5.5 Demonstration of spectral kernels against airborne reflectance data

The effectiveness of the spectral kernels to reconstruct spectral reflectance has been demonstrated. The final part of this experiment presents a brief example of the application of the spectral kernels (three soil and three vegetation) to airborne data over Barton Bendish, shown in figure 7.27. This demonstrates the possibilities for using the spectral kernels to generate spatial estimates of spectral model parameters.

The false colour composite (FCC) original ATM image shown at the top left of figure 7.27 forms part of multiple flight lines of data collected over the Barton Bendish area on various dates (described in section 3.1.5). These data are geometrically but not atmospherically corrected (due to a lack of information on atmospheric conditions during the overpasses, such as aerosol optical depth, water vapour and ozone concentrations). Pixel radiance values are weighted by a solar irradiance spectrum calculated for the date and time of the overpass. The inverted soil and vegetation parameters are also shown as FCC images i.e. first, second and third soil parameter on the red, green and blue channels respectively and the same for the vegetation parameters.

It can be seen in figure 7.27 that the soil parameters are bright where the original false colour composite ATM image is blue-ish, corresponding to soil areas and darker where there is likely to be vegetation (red in FCC). The third soil parameter is dominant over the farm area (see figure 3.1) which comprises harvested crops (stubble) and sugar beet. This behaviour contrasts with that over the airfield at the top of the image (areas covered by short grass and tarmac) where the first soil parameter is dominant. The vegetation parameters are generally bright where the likelihood of vegetated cover is highest in the original FCC image. The first parameter (and the third parameter to a lesser extent) is dominant except over the airfield, where the second parameter is bright resulting in a green colour. Interestingly, the RMSE image shows consistently lower values for areas of vegetation, than for bare soil. This figure demonstrates that there is significant information in spatial estimates of spectral model parameters, not only in
regard to differentiating areas of soil and vegetation cover but also in separating the spectral behaviour of different soil and vegetation types.

Figure 7.28 shows a scatter plot of original against modelled pixel values selected randomly from the original ATM image. Agreement between the two is high with an $r^2$ value of 0.96 when all bands are considered together. Individually, the only bands where
$r^2$ values fall below 0.9 are 435nm (possibly due to atmospheric scattering which is significantly higher at shorter wavelengths), 615nm and 830nm. The close agreement overall demonstrates the ability of the spectral kernels to describe spectral reflectance of soil and vegetation. In addition, the kernels appear to be capable of generating spatial estimates of soil and vegetation scattering components. This has far greater theoretical justification than an empirical estimate of vegetation such as NDVI and is nearly as rapid to apply. It will be straightforward to apply the full spectral directional kernel driven model to spectral directional reflectance data in the future, and use the resulting parameter values to interpolate estimates of narrowband albedo to broadband. This is discussed briefly in chapter 8.

![Figure 7.28 Scatter of original against modelled radiance values (using spectral kernels) for random points within ATM image of figure 7.27.](image-url)
7.6 Conclusion

It has been demonstrated that the concept of a spectral directional kernel driven model of \( \rho_{\text{canopy}}(\lambda, (\Omega, \Omega')) \) is feasible. Results indicate that such a model is likely to provide significant improvement over current kernel-driven models of directional reflectance, which operate independently of wavelength. It is shown that vegetation kernels derived from PCA of measured laboratory reflectance and transmittance spectra (combined as single scattering albedo) are capable of accurately describing spectral reflectance of a number of vegetation types. Some green vegetation spectra can be described adequately using only one vegetation kernel, but in most cases two or three kernels are necessary. In conjunction with two or three soil kernels, derived by Price (1990), it is shown that spectral canopy reflectance can be modelled very accurately. This approach is similar in some ways to linear unmixing (Settle and Drake, 1993), but differs in that the aim is to allow spectral interpolation of limited samples of reflectance, rather than the derivation of spectrally 'pure' end-members.

Results also show that the spectral kernels are highly effective in separating the constituent soil and vegetation components of spectral canopy reflectance. This is of significance for studies of photosynthetic activity (fAPAR), canopy efficiency and general vegetation influence, where it is desirable to be able to isolate the contribution of the vegetation component to total \( \rho_{\text{canopy}} \). The vegetation spectral kernels are particularly successful for canopies with LAI > 0.5. Even with only two or three vegetation spectral kernels it is likely that the majority of the single scattering contribution of vegetation reflectance to \( \rho_{\text{canopy}}(\lambda) \) can be extracted in most cases. The implication is that in cases where limited spectral sampling is available (e.g. MISR data, with only four bands), the kernels can act as spectral interpolants to generate full spectrum estimates of reflectance.

The spectral kernels can be simply combined with the directional kernels discussed in previous chapters to provide a full spectral, directional kernel-driven model of \( \rho_{\text{canopy}}(\lambda, (\Omega, \Omega')) \). Inversion of this type of model against simulated reflectance data indicates that full spectrum reconstruction of spectral directional reflectance from limited spectral directional samples is very accurate. As an example, reconstruction from selected MODIS wavebands is demonstrated. Derived spectral model parameters may well contain directional information, similar to the spectral information contained in the derived angular parameter values seen in chapter 6.
The success of the spectral kernels in reconstructing spectral reflectance confirms their utility as spectral interpolants, although much further validation is required in order to confirm their applicability. This will be of use for converting narrowband to broadband albedo and this will comprise the main direction for further research based on the spectral kernels. The next stage will be to test the kernels on aerial and spaceborne reflectance data in order to produce full shortwave spectrum reconstructions of reflectance data from limited spectral samples (an example of the spectral kernels' ability to describe spatial estimates of surface scattering and separate soil and vegetation scattering components is shown). These will then be used to generate shortwave albedo from airborne and spaceborne remote sensing data. A full spectral directional kernel-driven model can then be inverted against remotely sensed directional spectral reflectance data, such as that currently being produced by the MODIS instrument. Shortwave albedo can then be compared with the current operational MODIS albedo product. It is foreseen that the spectral directional kernel-driven model will greatly reduce the need for assumptions regarding atmospheric state and instrument band pass behaviour when interpolating narrowband samples of directional reflectance to produce broadband albedo. This is discussed in more detail in chapter 8.

Recent follow-up work by colleagues on the spectral kernels has indicated that it may be more effective to separate fresh and dry reflectance and transmittance spectra when generating the kernels in order to generate separate fresh and dry kernels (Collings, 2001). Using a suite of kernels in this manner (using the best fitting for a given circumstance) may be operationally feasible given that the computational overhead of inversion is very small. This is equivalent to the original AMBRALS (Algorithm for MODIS Bidirectional Reflectance and ALbedo) algorithm proposed for MODIS processing (Wanner et al., 1997), where a range of angular kernel combinations are inverted against each reflectance sample.

The final chapter sums up the results presented in this thesis, highlighting the most significant results. Areas related to this work where research is currently progressing are described, particularly in regard to the extension and application of the spectral kernels as part of a full spectral directional kernel-driven model. Suggestions are also made for where future research related to these topics might be directed.
8 Conclusions and directions for further work

8.1 Exploring the concept of linear kernel-driven models

This thesis sets out to explore the assumptions underlying the development and application of linear kernel-driven models of BRDF. The simplified semi-empirical approach to modelling $\rho_{\text{canopy}}$ underlying such models is examined, as is their potential for extracting biophysical information from reflectance data. Results presented here show that the linear kernel-driven models largely conform to the assumptions made in their formulation. In particular, evidence indicates that it is often justifiable to consider canopy scattering as a linear combination of volumetric and GO scattering components. This justification is less clear-cut in cases where the canopy departs markedly from the assumptions made in the kernel-driven models, particularly in a structural sense (strongly clumped, non-spherical LAD etc.). It has also been demonstrated that the volumetric and GO kernels are, in general, linearly related to the volumetric and GO components of canopy scattering, as would be expected if the kernels operate as intended. The relationship is generally much stronger for the volumetric component than for the GO component. This relationship has not previously been established quantitatively. In the past, the fact that the linear kernel-driven models tend to fit observed reflectance well has been used to justify their simplified nature.

Detailed 3D structural models of vegetation based on field measurement of canopy structure were used to simulate barley and wheat $\rho_{\text{canopy}}$ over a growing season. Validation against measured data indicated that the models represented the radiometric response of the vegetation reasonably well. Variation between measured and modelled reflectance values was due to variability in both field measurements and intra-field crop density. Simulations of $\rho_{\text{canopy}}$ were carried out under the same assumptions made in the formulation of the kernel-driven models i.e. independently of wavelength and considering only single scattering interactions and using a Lambertian soil surface.

The linear kernel-driven models assume that $\rho_{\text{canopy}}$ can be treated as separate (purely geometric) volumetric and GO components. In practice, these components are described using a linear superposition of separate volumetric and GO kernels (with an isotropic brightness term representing the multiple scattering contribution). Simulated $\rho_{\text{canopy}}$ was separated into its constituent volumetric and GO components. The volumetric component, related to scattering from vegetation only, was shown to behave as expected
for vegetation reflectance. The GO component (related to the proportion of visible sunlit soil in this case) does not agree precisely with expectations, in that a hotspot feature was not apparent due to the departure of the canopies used in the experiments from the ideal GO canopy visualised in the formulation of GO models of CR. The respective volumetric and GO canopy components were shown to change with the developing canopy as expected during the growing season. The volumetric component increased with increasing LAI until the canopy reached senescence. Conversely, the GO component reduced over time as a result of the soil becoming obscured by the developing vegetation.

Two fundamental hypotheses were presented, both of which must hold true for the kernel-driven models to be valid. Firstly, it must be possible to describe $\rho_{\text{canopy}}$ as a linear combination of separate volumetric and GO terms. Results showed that in many cases this hypothesis was true, with strong linear relationships between the volumetric and GO scattering components and their respective kernels. However, there was significant variation, particularly in the relationship of the GO component to $k_{\text{GO}}$, the GO scattering kernel. This is a result of the fact that the GO component being modelled is significantly different from the theoretical GO component of $\rho_{\text{canopy}}$ envisioned in the kernels (Li and Strahler, 1985, 1986; Wanner et al., 1997), in particular, the canopy is composed of many relatively small leaves rather than scattering 'spheroids-on-sticks' (see 2.5.4.1.2).

The agreement between the scattering components and their respective kernels was particularly noticeable in canopies with one dominant scattering component. The assumption broke down in more extreme cases when either there was very little vegetation present (and hence virtually no volume scattering) or else the canopy had senesced, with little green vegetation remaining. In these cases the canopy had diverged even further from the general assumptions of the linear models. Departure from the assumption of spherical LAD was shown to have a significant impact on the relation of the volumetric and GO components of canopy scattering to the respective model kernels. The tendency of agricultural canopies to have regular planting patterns exacerbates this by violating the assumption of azimuthal invariance. This can lead to significant clumping, particularly at early stages of growth. This appeared to impair the ability of the models to describe the reflectance of this type of canopy. Forests also tend to have non-uniform distributions of vegetation and/or LAD and may pose similar problems.

The second hypothesis examined was that the volumetric and GO components of
\( \rho_{\text{canopy}} \) can be described adequately by the volumetric and GO kernels alone. Results indicated that this hypothesis is true in some cases, with the individual scattering components of \( \rho_{\text{canopy}} \) being largely separable. Again, discrepancies tended to occur where the canopy departed from the assumptions of azimuthal invariance and spherical LAD. In these cases it was clear that some proportion of volumetric scattering was explained by the GO kernel, while conversely, some GO scattering was taken up by the volumetric kernel. This indicated an element of coupling between the kernels. The implication is that model parameter values need to be interpreted very carefully in practice. In cases where the vegetation canopy departs from the (structural) assumptions underlying the kernel-driven models it will not be possible to relate the model parameters directly to their respective scattering components.

Spectral estimates of the angular kernels were derived. As expected, the volumetric kernel tended (spectrally) to resemble \( \rho_{\text{leaf}} \) and the GO kernel resembled \( \rho_{\text{soil}} \). In some cases the respective kernels clearly contained information regarding the other scattering component. In particular, the isotropic kernel appears to be correlated with \( \rho_{\text{leaf}} \) in some cases. As the canopies developed, the volumetric and GO parameters increasingly resembled each other, indicating an increased degree of coupling as well as the difficulty of separating the components in these cases. As a consequence it may not be possible to interpret parameter values directly without ancillary data, such as estimates of \( \rho_{\text{leaf}} \). This may not be practical in many cases, for example in applications involving moderate resolution data with large areal coverage (thousands of km\(^2\)).

In nearly all cases the RossThick LiSparse kernel combination was the best fit to observed reflectance, supporting the choice of this combination as the primary model for processing MODIS reflectance data. The behaviour of the spectral estimates of the angular kernels indicates that they may be suited to classification of reflectance data, as they might be used as extra channels of information regarding scattering from soil and vegetation. In particular, the model parameters may be able to separate soil and vegetation scattering components, which will prove useful for studies of carbon budget, fAPAR and NPP. It was noted that, in some cases, derived values of the model parameters could take physically unrealistic (negative) values. This is not a problem if the parameters are to be used for classification for example, as in this case it is simply the relative values that are important. However, if the parameters are to be interpreted then inversion should be constrained so that parameter values are physically realistic.
8.2 Extension of the kernel-driven modelling concept

The linear kernel-driven models are based on the idea that simple volumetric and GO 'shape' terms can be combined to describe the dominant angular features of surface BRDF. This concept was adapted and extended into the spectral domain based on the observation that vegetation (and soil) spectral reflectance displays a number of common features. There are a number of benefits that a combined spectral directional kernel-driven model of ρ_canopy confers. Chief amongst these is the ability to interpolate narrowband samples of reflectance over a wide range of wavelengths. This is analogous to the application of the angular kernels to interpolate/extrapolate limited directional samples of reflectance to arbitrary viewing/illumination angles. This ability to interpolate (and possibly extrapolate) narrowband reflectance samples would be extremely useful in deriving albedo, which typically requires assumptions to be made regarding spectral weightings of narrowband reflectance samples and the shape of the solar spectrum. A spectral kernel-driven model will obviate the need for such assumptions. Another benefit is the ability to separate the spectral components of scattering from soil and vegetation. This is of particular importance in studies of fAPAR and NPP, where only scattering from vegetation is of interest. A further advantage is that spectral kernels will permit the combination of data from sensors with different bandpass functions. Spectral kernels could be used to 'normalise' spectral reflectance to some common set of wavebands. This is analogous to normalisation of directional reflectance to specified viewing and illumination angles (typically nadir) using the angular kernels.

Based on previous work deriving soil basis functions (or spectral kernels), a number of vegetation spectral kernels were derived from measured reflectance and transmittance spectra. It was demonstrated that three or four of these spectral kernels are sufficient to describe greater than 98% of observed variance in a large range of measured vegetation spectra. It was shown that a combination of five or six soil and vegetation kernels were able to describe observed spectral ρ_canopy extremely well. In some cases as little as two or three spectral kernels in total were required to adequately fit observed data. This is likely to be sufficient for many multispectral sensors, which tend to have four or more spectral bands. The spectral kernels were applied in conjunction with angular kernels to simulated values of spectral directional ρ_canopy. The full spectral directional kernel-driven model fitted the simulated reflectance values extremely well, with RMSE of < 4% in all cases. In cases where three soil and three vegetation kernels are used, RMSE
of fit falls to between 0.1% and 1%. The kernels were also shown to be capable of separating soil and vegetation spectral components of $\rho_{\text{canopy}}$ successfully. Spectral estimates of the angular kernels were derived which illustrated that some angular information was contained in the spectral kernels. Full spectrum reconstruction of spectral reflectance from limited (MODIS) wavebands also showed the success of the spectral kernels. These results indicate that the spectral directional kernel-driven model is likely to provide significant improvement over current kernel-driven models of directional reflectance, which operate independently of wavelength. Further work is needed to explore the ability of the kernels to generate albedo but initial results suggest they may be very effective.

### 8.3 Directions for future research

The work presented in this thesis is part of ongoing research into the scattering behaviour of vegetation canopies and how this behaviour can be modelled and hence exploited. However, there are several specific areas in which the work in this thesis will be built upon and extended and these are briefly outlined below.

#### 8.3.1 Application of full spectral, directional kernel-driven model

A full spectral directional linear kernel-driven model is under development. This will be applied to airborne thematic mapper (ATM) and compact airborne spectrographic imager (CASI) data obtained over the Barton Bendish site in 1997. ATM data are limited to 11 visible and NIR wavebands, whilst CASI has up to 288 bands (depending on the chosen configuration). It is proposed that the spectral kernels be used to reconstruct the CASI data spectrally from the ATM data. This will provide an excellent test of the spectral kernels ability to model spectral reflectance. Once these data are atmospherically and geometrically corrected to the required accuracy (sub-pixel registration accuracy is required for BRDF studies) they will be used to derive broadband albedo. These values will then be compared with MODIS albedo estimates over the same area. This will provide a link between high resolution albedo derived from the airborne data and the moderate resolution (km scale) MODIS product, contributing to ongoing MODIS validation work (www[8.1]). Validating albedo is difficult given that field-measured
albedo is typically a point measure from an albedometer and relatively few samples can be collected over areas covered by even a very small number of MODIS pixels (Lucht et al., 2000). The spectral kernels will also be used to generate spatial estimates of soil and vegetation spectral and directional reflectance components (as in section 7.5.5). These will be compared with estimates derived from field measurements. If this is successful it will demonstrate the use of the spectral kernels for applications requiring scattering information from vegetation alone.

It is intended that the full spectral directional kernel driven model be applied to the spectral directional reflectance data as described above and that the resulting parameter values be used to interpolate estimates of narrowband albedo to broadband. This has typically been a laborious process requiring a number of approximations and assumptions (see chapter 2). Conversion of narrowband to broadband albedo will be carried out once the ATM and CASI airborne data have been pre-processed to the required accuracy. This includes sub-pixel geometric correction required for BRDF model inversion (Barnsley et al., 1997) and accurate atmospheric correction based on the MISR algorithm of Martonchik et al., 1998a). In addition, data from the CHRIS mission (launched in October 2001 aboard the PROBA platform) will be available for comparison with airborne estimates of albedo. CHRIS is a pointable high resolution optical instrument with selectable bands (www[1.11]). It is anticipated that the spectral directional kernel-driven models will be ideal for inversion against CHRIS data. Estimates of albedo (and biophysical parameters) can then be compared directly with MODIS products over the same area. It is expected that this will provide better understanding of the issues involved in scaling albedo from ground-based, to moderate resolution data.

8.3.2 Other canopy types

Much of the work in this thesis is intended as a benchmark for the application of the kernel-driven models, as well as an indication of the information it may be possible to derive from their parameters. The methods employed here can be used in the future to test modifications to the kernels and try out new formulations. In addition, it is now possible to simulate the reflectance of forest canopies using the explicit 3D geometric BPMS model (given suitable field measurements). It is likely to be an interesting and worthwhile
exercise to apply the methods used in this thesis to such different canopies. This would
give a more direct indication of the applicability of the kernel-driven models to a wide
range of land cover types.

A further possibility is to construct detailed 3D models of the GO and volumetric
scattering arrangements postulated in the kernel-driven models. In the case of the GO
kernels this requires constructing arrangements of 'spheroids on sticks'; the volumetric
kernels require approximating the horizontally homogeneous scattering 'cloud'. It would
then be possible to explore what size and shape of scattering objects and/or combinations
most closely correspond to 'real' plant canopies. Figure 8.1 shows an example of this
approach carried out as part of the RAMI exercise (Pinty et al., 2001). This is a
simulation of a vegetation canopy with spherical 'clumps' of vegetation of fixed LAI,
comprised of randomly located disks with specified LAD.

Figure 8.1 Simulated 'vegetation' canopy
8.3.3 Multiple scattering

The assumption of single scattering interactions made in the formulation of the kernel-driven models has (intentionally) received little attention in this thesis. It is clear that single scattering interactions do dominate $\rho_{\text{canopy}}$, particularly in the visible part of the spectrum (see figure 7.1). However, this is not necessarily the case in the NIR where reflectance is much higher. Application of the spectral kernels over the wider spectrum means that multiple scattering is likely to become more important. It may also be possible to derive information regarding the canopy structure from analysis of multiply scattered information. It is known that there are approximations that can represent multiple scattering reasonably well (Knyazikhin and Marshak, 2000). If this information can be modelled using relatively simple terms it may be possible to construct a kernel-driven expression for the multiple scattering component, rather than lump it in as 'brightness' term as is currently the case in the kernel-driven models. An advantage of this is it may lead to a better description of $\rho_{\text{canopy}}$. In addition, the multiple scattering component is known to contain information regarding canopy structure, which it may be possible to extract.

Some analysis of the multiple scattering component of $\rho_{\text{canopy}}$ from the canopies used in this thesis has already been attempted (Disney and Lewis, 1998). This work has shown that there may be a simple approximation for describing multiple scattering as a function of scattering order within the canopy. This may not be so important for studies of albedo, due to differences in scattering behaviour between the visible and SWIR regions: single scattering dominates in the visible, whilst multiple scattering dominates in the SWIR and NIR. Visible radiation has a larger impact on shortwave albedo than SWIR and NIR, as around 40% of total solar energy arriving at the surface lies between 0.3 and 0.8μm (see figure 1.3). However, a simple approximation for representing the multiple scattering component of $\rho_{\text{canopy}}$ is likely to be useful for deriving biophysical information. Lewis and Disney (1998) have shown that such an approach is very similar to theoretical work by other groups based on solutions to the 3D radiative transfer equation in a vegetation canopy (Knyazikhin, pers. comm.). It is intended that studies of multiple scattering will be fully incorporated into future analysis of kernel-driven BRDF modelling, again through the use of full 3D structural models of vegetation.
8.3.4 Improved fieldwork measurements

The fieldwork described in chapter 3, intended to validate canopy radiometric simulations, was subject to a number of problems. Chief amongst these was poor weather, which (unfortunately) cannot be legislated for. However, part of ongoing research into linear kernel-driven models of $\rho_{\text{canopy}}$ will be to refine the methods used here in an effort to generate a significantly better set of fieldwork measurements. Following the fieldwork of 1997, it is much easier to determine what needs to be measured in the future, how accurately these measurements can be expected to be, and how existing measurements may be improved.

The scope and detail of what can be measured is partly determined by available manpower. Most of the measurements used in this thesis were carried out by two groups of two people (often less). This severely restricts the degree of spatial sampling that can be carried out as well as the overall number of parameters which can be measured. However, within these limitations, a number of improvements can be made. Firstly, radiometric measurements can be carried out using a larger FOV ($15^\circ$) radiometer head. The advantage of this is that it is not as sensitive to the pointing accuracy of the radiometer (a few degrees at best). The disadvantage of this is that features of measured BRFD such as the hotspot will become 'smeared out'. However, for validation it is more important to characterise the general magnitude and angular variation of BRDF than to measure features such as hotspot width, say.

Another way of significantly improving future field radiometric measurements is with the use of a sun photometer to characterise atmospheric scattering. This is vital not only for ground-based radiometric measurements (seen figure 3.7), but also for atmospheric correction of airborne and satellite remote sensing data. One of the difficulties of processing the airborne data collected in 1997 has been the lack of contemporaneous measurements of atmospheric aerosol and water vapour properties. This is considered essential for studies of BRDF (and hence albedo). A CIMEL (www[8.2]) sun photometer has been made available for fieldwork at Barton Bendish, as part of the NASA Aerosol Robotic Network (AERONET, www[8.3]) and general MODIS validation effort. This will allow accurate characterisation of atmospheric scattering during future campaigns. Walthall et al. (2000) describe a number of protocols including angular and spatial sampling regimes and atmospheric measurements which are generally accepted as
essential in field measurement of BRDF. These protocols will be adopted for future fieldwork. Finally, in order for useful comparisons to be made between spatial albedo values generated at high spatial resolution (e.g. from airborne data) and satellite-derived values, some validation at the surface is required. The use of an albedometer through the growing season would achieve this. It is limited essentially to point measurements, but if large, relatively homogeneous (at the field scale), fields of barley and wheat are used, the albedo can be assumed to be fairly constant over a whole field. This would provide the required link between albedo generated from airborne and spaceborne using the spectral kernels and albedo measured (and simulated) at canopy scale.

8.3.5 Optical and microwave scattering

One final, broad area where the work carried out in this thesis will be continued and extended is the marrying of scattering in vegetation in the optical and microwave domain. Currently, physical descriptions of scattering these two domains are very different. This is because the dimensions of canopy scattering objects (such as leaves) are far larger than optical wavelengths, but typically of the same order of magnitude as microwave radiation (λ of mm to cm). This leads to a number of problems for those constructing models of canopy scattering in this domain, in particular the consideration of absorption and scattering at the leaf level. It is not a simple matter of reflectance, transmittance and absorptance behaviour as in the optical domain. Nor can useful simplifications such as Lambertian scattering be applied. In microwave models of canopy scattering, gross simplifications are required such as the use of 'equivalent disks' to represent leaves, and cylinders representing stems. Complex phase scattering matrices and assumptions about dielectric behaviour are required to solve even these cases. However, the fundamental representations of canopy structure are the same. It may be possible to apply the type of assumptions regarding simple scattering 'shapes' made in the kernel-driven models to microwave backscatter models. This would prove extremely useful, given the advantages that RADAR instruments hold over optical ones in being able to penetrate cloud and operate on the Earth's dark side. It has already been recognised that the conceptually different approaches to modelling of vegetation in the optical and microwave domains are in fact linked by a common need to consider vegetation structure (Saich et al., 2001). It is intended that methods developed in this thesis will be applied to examining possible linkages between microwave scattering and the kernel-driven approach to modelling canopy reflectance in the optical domain.
Appendix 1

Constraint of linear model parameters for inversion (Lewis, *pers. comm.*)

The inversion of linear kernel-driven BRDF models against measured reflectance data can, in practice, result in model inverted parameter values that are physically unrealisable (Strugnell and Lucht, 2000). This tends to occur when a chosen kernel combination cannot describe surface reflectance adequately. There are two reasons for this failure. Firstly, the selected kernel combination may simply be inappropriate for the cover type under observation. This typically occurs in areas where the surface may be at the extremes of what was envisioned in the kernel formulation e.g. sparse canopies over very bright/rough soils; canopies with extreme LAD (departure from spherical assumption of volumetric kernels); dense forest canopy where the assumptions of discrete crown and ground areas break down. Secondly, there may be insufficient information in the signal (variation related to surface structure in the reflectance data) for a full linear model comprising an isotropic, volumetric and GO kernel, to be inverted, hence the best-fit solution (lowest RMSE) may be physically unrealistic.

If the parameters are to be used indirectly e.g. as an additional channel of information for classification (beyond the spatial and spectral) then the absolute values are not important, only the spatial variations. As demonstrated in chapters 5 and 6, inverted linear model parameters do contain biophysical information related to the volumetric and GO scattering properties of a surface, and this is the important issue for indirect use. If parameters are to be used directly however e.g. to extrapolate/interpolate directional reflectance values, or to derive associated surface properties such as directional hemispherical reflectance or spectral albedo, then clearly it is sensible to place physical constraints on the derived properties. These constraints can then be used to direct the inversion procedure.

Recall from section 2.5.4.1 that a linear model of BRDF can be represented as $\rho_{\text{canopy}} = f_0 + f_1 k_1 + f_2 k_2$. Recall also that the unconstrained inversion of such a model against a set of observations over varying $k_1$, $k_2$ is simply the minimisation of $e^2$, the sum squared error between modelled and measured reflectances i.e.
which results in a series of linear equations, one for each observation. This can be simply solved using matrix algebra (see section 2.4.1.1, after Lewis, 1995) i.e. $P = M^{-1}V$ where

$$V = \frac{1}{N} \sum_{i=1}^{N} (\rho_i - (f_0 + f_1k_i + f_2k_i^2))^2$$

and

$$M = \frac{1}{N} \sum_{i=1}^{N} \begin{bmatrix}
1 & k_{ii} & k_{2i} \\
k_{ii} & k_{ii}^2 & k_{i1k_{2i}} \\
k_{2i} & k_{2i}k_{ii} & k_{2i}^2
\end{bmatrix}$$

Lagrange multipliers can be applied to such a system to impose arbitrary constraints under which inversion may be carried out. Lagrange multipliers allow the minimum (or maximum) of a function $f(f_0, f_1, f_2)$ to be found by using a relationship between the function parameters and some constant i.e. $\varphi(f_0, f_1, f_2) = \text{constant}$ (e.g. Boas, 1983). In this case, the function $\varphi(f_0, f_1, f_2)$ is the constraint equation, based on some physical limits. $e^2$ can now be minimised based on the original model in addition to the constraint equation i.e. we wish also to minimise $\varphi = af_0 + bf_1 + cf_2 - d = 0$ or $C \cdot P = d$ where $C$ is the transpose of the matrix containing the Lagrange multipliers i.e. $C = (a, b, c)^T$ and the minimisation is now a function of the constraint equation in addition to the original expression i.e.

$$e^2 = \frac{1}{N} \sum_{i=1}^{N} (\rho_i - (f_0 + f_1k_i + f_2k_i^2))^2 - 2\lambda(af_0 + bf_1 + cf_2 - d)$$

Minimisation therefore leads to $V = MP + \lambda C$ and $V - \lambda C = MP$ and multiplying by the inverse of $M$ i.e. $M^{-1}V - \lambda M^{-1}C = P$ or $P' - \lambda C' = P$ where $P' = M^{-1}V$ and $C' = M^{-1}C$, and $P'$ is the parameter values obtained from unconstrained minimisation. Now, clearly $P' \cdot C - \lambda C' \cdot C = P \cdot C$ and we have already seen that $C \cdot P = d$, so that we can derive an expression for $\lambda$ i.e.

$$\lambda = \frac{P' \cdot C - d}{C' \cdot C}$$
and since we know that $M^{-1}V - \lambda M^{-1}C = P$ then

$$P' = \left( \frac{P' \cdot C - d}{C' \cdot C} \right) C' = P$$

A 1.6

i.e. if $M^{-1}$ and $P'$ are calculated in an unconstrained manner then the inverse matrix can be multiplied by the constraint vector $C$ to obtain $C'$, and hence $P$, the set of constrained parameters, can be calculated. Practically the difficulty is to find a constraint equation that relates the model parameters to some constant. The most obvious physical constraint is that the surface reflectance should be $\geq 0$. In this case, we can say that $f_0, f_1, f_2 \geq 0$ i.e. $f_0 + f_1 + f_2 \geq 0$ and $f_0 + f_1 k_1 + f_2 k_2 \geq 0$. Furthermore, it seems sensible to constrain the DHR and for both the maximum and minimum kernel values, to lie between 0 and 1 i.e.

$$0 \leq f_0 + f_1 k_1(0) + f_2 k_2(0) \leq 1$$

A 1.7

$$0 \leq f_0 + f_1 \bar{k}_1 \left( \frac{\pi}{2} \right) + f_2 \bar{k}_2 \left( \frac{\pi}{2} \right) \leq 1$$

A 1.8

In which case it should also be reasonable to constrain the BHR to lie within the same limits i.e. $0 \leq f_0 + f_1 \bar{k}_1 + f_2 \bar{k}_2 \leq 1$. Constraint requires the calculation of the unconstrained parameters followed by a test of the various products against each constraint in turn. If any constraint is not met, all constraints should be applied. Following re-calculation of the constrained model parameter sets, RMSE can be used to select a single, final set of values. Although this may seem arbitrary, it requires no \textit{a priori} assumptions to be made about which constraints the model “should” and “should not” adhere to. The requirement for speed may be what limits the application of constraints in practice, although the number of extra calculations required for each constraint is not prohibitive.

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1 Although individual constraints could be used, this is probably not physically very sound. If just one of the constraints is not met, we can must conclude that the inversion is misbehaving.
Appendix 2

Figure A2.1 Proportional contribution of sunlit and shaded scene components to total scene reflectance, for barley (four dates) and wheat (two dates).

a) barley – 18th April

b) barley – 13th May
c) barley - 4\textsuperscript{th} June

d) barley - 24\textsuperscript{th} June
c) wheat – 23rd March

d) wheat – 23rd April
Sunlit and shaded scene components of barley and wheat

The results presented in figure A2.1 should be compared with those in figure 4.7, which were generated using no diffuse component of illumination, and hence have no contribution to overall scene reflectance from the shadowed canopy components. The reflectance and transmittance in each case are the same i.e. two 'synthetic' wavebands are simulated, the first in which \( \rho_{\text{leaf}} = \tau_{\text{leaf}} = 0.5 \) and \( \rho_{\text{soil}} = 0 \) i.e. in this case all signal is (by definition) scattering from vegetation only (only single scattered interactions are counted); the second waveband has \( \rho_{\text{leaf}} = \tau_{\text{leaf}} = 0 \) and \( \rho_{\text{soil}} = 1 \) i.e. in this case all signal is (by definition) single scattering from soil only. Results are presented from \( \theta_s = 0^\circ, 30^\circ \) and \( 60^\circ \), as well as for \( \phi_{\text{row}} = 0^\circ, 45^\circ, 90^\circ \). Separation of the different \( \phi_{\text{row}} \) cases increases with LAI. It can clearly be seen in figure A2.1a, for example, how the sunlit leaf is at a maximum in the hotspot (\( \theta_s = \theta_v = 0^\circ \)) and shadowed soil is a minimum (close to zero).

It can be seen that in these cases, the sunlit soil is the dominant scene component in both low LAI cases (figure A2.1a and e), particularly in the 23rd March wheat canopy. In this case the sunlit soil component represents greater than 80% of the total reflectance at all \( \theta_{v,i} \) with all other components representing less than 10%. For barley the contribution of other components, sunlit leaf in particular, is significant.
References


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