

**CO Spectral Line Formation in the Sun:
Convective Simulation, Line Profiles and Isotopic
Abundance Measures**

Patrick C. Scott



THE AUSTRALIAN NATIONAL UNIVERSITY

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Declaration

This thesis is an account of research undertaken between February and October 2004 at The Research School of Astronomy & Astrophysics, The Australian National University, Canberra, Australia.

Except where acknowledged in the customary manner, to the best of my knowledge the material presented in this thesis is original and has not been submitted in whole or part for any degree at any university.

Patrick Scott
October, 2004

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Abstract

CO spectral line formation in the Sun was modelled using realistic, ab initio, time-dependent 3D radiative-hydrodynamical model atmospheres. Three ‘phases’ of 3D model atmospheres were utilised. In Phase 1, strong CO lines formed in very high atmospheric layers were modelled using the established model (Asplund et al. 2000b). This produced less than perfect agreement with observed line asymmetries measured in the ATMOS disc-centre solar atlas. The velocity, temperature and density fields were then manually altered during Phase 2 in order to ascertain the reasons for the disagreement with observation during Phase 1. Following reasonably successful reproduction of observed profiles and bisectors in Phase 2, new self-consistent simulations were performed using an updated version of the hydrodynamical code and an extended simulation domain in Phase 3. In this final phase, excellent agreement between observed and synthesised line profile shapes, depths and bisectors was achieved.

Using different sets of weak $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ lines from the fundamental ($\Delta\nu = 1$) band, the solar carbon abundance, $^{12}\text{C}/^{13}\text{C}$ and $^{16}\text{O}/^{18}\text{O}$ isotopic ratios were also determined. In addition, two alternative $^{12}\text{C}^{16}\text{O}$ line lists, one of low excitation potential and one of first overtone transitions, were analysed for comparison with the weak $^{12}\text{C}^{16}\text{O}$ lines. A solar carbon abundance of $\log \epsilon_{\text{C}} = 8.40 \pm 0.04$ was found. We note with satisfaction that the derived abundance is almost identical to the recent 3D determination of Asplund et al. (2004a) using permitted and forbidden atomic carbon lines, as well as CH and C₂ molecular lines. This increases our confidence in the accuracy of both results. No trends with equivalent width, excitation potential or wavelength were evident in the 3D results, except in the case of the stronger low excitation lines. Identical calculations were carried out using 1D models, but only the 3D model was able to produce abundance agreement between different CO lines *and* the very different carbon diagnostics of Asplund et al. (2004a). For example, had the 1D Holweger-Müller model been used instead, the derived C abundance would have been 0.14 dex higher. Solar $^{12}\text{C}/^{13}\text{C}$ and $^{16}\text{O}/^{18}\text{O}$ ratios were measured at $93.8^{+8.0}_{-7.6}$ and 523^{+60}_{-55} respectively. These values are in good agreement with the terrestrial ratios, and present a significant improvement upon the previous ratios of Harris et al. (1987). The corresponding 1D-based ratios are significantly lower, differing markedly from the telluric values.

The successful model atmosphere indicates the existence of a $\sim 4000\text{K}$ COmosphere around the traditional temperature minimum, with cool CO extending in significant concentration to approximately 700 km above the surface. However, the presence of even cooler localised regions is crucial in producing agreement between synthetic and observed CO lines, due to the extreme temperature sensitivity of the CO molecule. This result does not preclude the existence of cool gas at heights greater than about 700 km, which are not probed by the lines studied here.

Despite these successes, simulations were seen to marginally overpredict temperatures very high in the atmosphere, though the temperature structure at all but the greatest atmospheric heights appears very accurate. This minor deficiency in the 3D model atmospheres was identified as an avenue for their future improvement.

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Introduction

1.1 Overview

As the only star in our vicinity, the Sun is without peer as a laboratory for the study of stellar physics. It is undoubtedly the star from which we possess the greatest amount of observational data. This depth of information provides the opportunity to scrutinize and refine relevant theory to a considerably more detailed level than is usually possible in astrophysics. Such resolution also allows for far more accurate determination of solar quantities than is common in astronomy.

Despite the multitude of data, nobody would dare claim that we fully comprehend the Sun (see Kurucz 2002, for one account of gaps in our current understanding). As is the case with almost any physical system or phenomenon, the more we understand, the more we realise we don't. As it is with the Sun; as we have unravelled its basic structural and evolutionary properties (discussed in §1.1.1), so more complex unsolved problems such as helioseismology (e.g. di Mauro 2003), coronal processes (e.g. Galsgaard et al. 2000) and convection are now being dealt with. It is in these comparably smaller-scale realms that the Sun's wealth of observational data really comes into its own.

The latter of these fields is the one with which this study is associated: convection. The Sun's gross internal structure is illustrated in Fig. 1.1. The existence of this structure and its described properties are justified in §1.1.1. Radially speaking, approximately the inner fifth of the Sun is the thermonuclear core currently powering the star via hydrogen burning, shown in the diagram as a very dark region. Energy transport in this region is predominantly radiative, as it is in the lighter shaded region extending from the core to about two thirds from the centre. The upper third of the Sun's radius however, is dominated by convective energy transport. This means that the temperature gradient with respect to height from the solar core is so steep in this region, and the mean free path of photons so short that energy transfer will occur more efficiently by gas actually itself moving to the surface of the star, than by the photons it emits. The result is an upper layer of the Sun that bubbles like a pot of boiling water, as can be seen in the enlarged section of Fig. 1.1. This is the famous 'granulation pattern' seen on the solar surface. As the reader will see, convection is an exceedingly complex, nonlinear process and as such is only recently beginning to be dealt with effectively (Stein & Nordlund 1998; Asplund et al. 2000b).

Convective transport in the upper layers of the Sun has a large bearing upon absorption and emission lines produced in its atmosphere (Asplund et al. 2000b; Uitenbroek 2000a), so any analysis involving such lines must generally take convection into account. Indeed, virtually everything we know about the Sun is derived from spectral analysis, so the importance of proper treatment of convection is clear. One particularly important

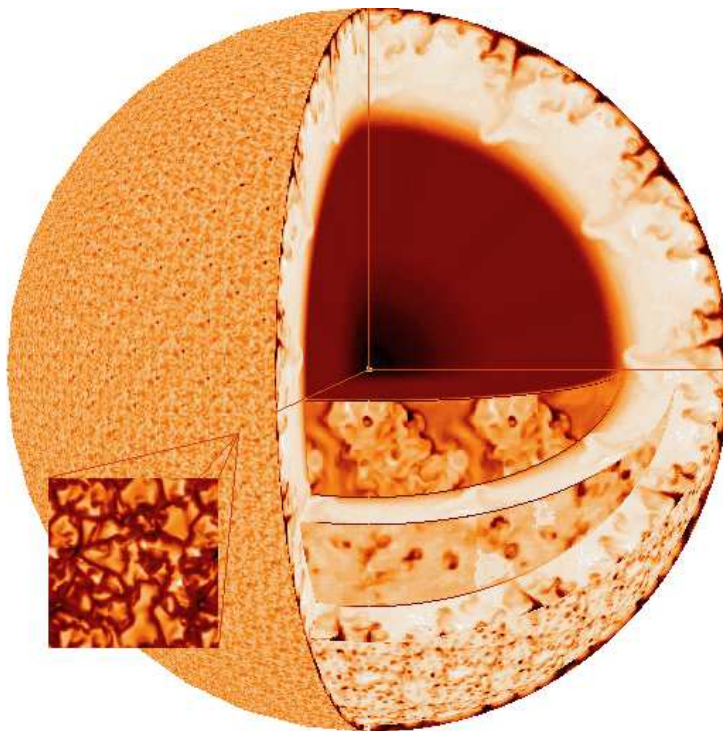


Figure 1.1: Our Sun, showing a cutaway view of the basic interior structure. Note the dark nuclear burning region in the inner fifth and the convective envelope over the outer third of the total radius. The inset frame shows an enlarged section of the surface, illustrating the granulation pattern of convection. (Figure obtained from Nordlund 2004)

procedure is the measurement of relative abundances of elemental and molecular species present in the Sun. The results of such analyses have far-reaching implications for cosmological, interstellar and planetary physics (Asplund et al. 2004c; Langer & Penzias 1993), so accuracy in their execution is paramount.

A notoriously difficult chemical species to perform any kind of solar analysis with is carbon monoxide (CO) (Uitenbroek 2000a). No published model of the solar atmosphere has claimed to completely describe CO line formation. Debate has raged (e.g. Ayres 2002; Kalkofen 2001) for some time as to what CO absorption features in the solar spectrum are in fact telling us. In particular, questions remain over the location of CO in the solar atmosphere and the associated atmospheric temperature structure. In studying CO line formation in the Sun using the latest in convective model atmospheres, we¹ hope to at last answer these questions conclusively.

1.1.1 The Standard Model of Stellar Structure and Evolution

The basic structure of the Sun shown in Fig. 1.1 is a result known from the **Standard Model** of stellar structure and evolution (Carroll & Ostlie 1996). This model is something of an emergent consensus over the past 100 years as to the fundamentals of stellar astrophysics. The model describes pressure, temperature, luminosity and mass as a function of radius in a spherically symmetric star. The nuts and bolts of the model (Carroll & Ostlie 1996; Stix 2002) are four coupled first order differential equations relating the four quan-

¹‘we’ being the author Patrick Scott and supervisor Martin Asplund

ties, with corresponding boundary conditions. The complexity in such models comes from the dependence of the differential equations upon four other variables, producing the need for further **constitutive relations**, often collectively referred to as the **equations of state**. These equations of state describe energy, opacity, entropy and density in terms of the primary variables of the differential equations, closing the system and therefore allowing solution. The algebraic form of the differential equations and which thermodynamic variables the constitutive relations are expressed in terms of varies (e.g. Kippenhahn & Weigert 1991; Bisnovatyi-Kogan 2001; Chandrasekhar 1967), but they all represent fundamentally the same physical model (at least to first order). The actual physical content of the equations of state can however be very complex, differing depending on the sophistication of the particular simulation carried out to reflect many different physical processes occurring in a stellar interior. They also typically differ depending upon a star's chemical composition, which is allowed to evolve in time as nuclear burning occurs. This permits the temporal evolution of the model. The known solar structure described earlier is the typical output of such a model run for a solar lifetime, using solar parameters.

The Standard Model will not be discussed in detail, nor its system of equations reproduced, as it is not itself the focus of this thesis. It does however provide an historical and broader theoretical context in which the atmospheric theory discussed in Chapters 2 and 3 sits, and the constitutive relations play a central role in the computational method of the work we describe.

1.2 Aims of the Investigation

We propose to investigate carbon monoxide (CO) absorption line formation in the solar spectrum using three-dimensional radiation-hydrodynamics simulations of the Sun's atmosphere. We will specifically study spectral line shapes and asymmetries, comparing the simulation output to the observed solar spectrum from the Atmospheric Trace Molecule Spectroscopy (ATMOS) space shuttle mission. With this comparison, we expect to gain further insight into the solar distribution of CO and the temperature structure of the solar atmosphere, two extremely contentious issues (e.g. Ulmschneider 2003; Ayres 2000). In doing this, we will assess how well the model atmospheres employed describe the troublesome CO molecule and thereby possibly also identify some areas for their refinement. Very few such 3D models have been applied to CO line formation, and those that have (Uitenbroek 2000a) were not as sophisticated as the one to be described Chapter 3. For this reason, we hope that this will be the first study and model to properly describe and explain CO line formation in the solar disc. We expect that if this is the case, it will then also provide a clear platform for later efforts to achieve the same in the vicinity of the limb of the disc.

We also aim to produce a series of new solar abundance determinations for isotopes of carbon and oxygen using the ATMOS data and the same model atmosphere. Specifically, we will arrive at new estimates of the solar carbon abundance and the $^{12}\text{C}/^{13}\text{C}$ and $^{16}\text{C}/^{18}\text{O}$ ratios. Whilst these quantities have been measured before (Harris et al. 1987), the analysis has never been made using modern 3D model atmospheres. We hence expect that our results will constitute a significantly more reliable and accurate measure than those of the past.

1.3 Thesis Structure

As a thesis, this document aims to give a thorough explanation of the theoretical and historical background drawn upon by the study as well as its execution and findings. As such, Chapter 2 gives something of a crash course in the traditional treatment of the solar atmosphere from opacity and optical depth to the layering paradigm, radiative transfer, spectral formation and finally the status quo in convective treatment: Mixing Length Theory. Those having had prior contact with stellar atmospheres will likely want to avoid this dirty phrase and begin at Chapter 3, which describes the structure, properties and recent results of the 3D radiative-hydrodynamical models to be employed. Throughout these two chapters, the focus will be almost exclusively on the Sun, but most of what will be said is equally applicable to other stars.

This is followed in Chapter 4 by an exposition of the rather thorny problem of solar CO and its debate over the past years. Chapter 5 relates the theory and methods of abundance determination by spectral line analysis, particularly in the current context of solar CO and the 3D model atmospheres to be employed. Chapter 6 describes the ATMOS experiment and our manipulation of its data. The study of the properties of CO absorption lines is described and discussed in Chapter 7, and the abundance and isotopic ratio determinations in Chapter 8. Conclusions, implications and possible future directions of this work are summarised in Chapter 9. Appendix A consists of a brief inventory of computational work carried out (rather than full code listings), and Appendix B contains full spectral line lists used.

Traditional Solar Atmospherics

2.1 Opacity & Optical Depth

The concepts of opacity and optical depth are integral to the description of stellar atmospheres, and as such should be explicitly defined at the outset. The explanations in this section draw on treatments in three standard texts (Carrol & Ostlie 1996; Stix 2002; Kippenhahn & Weigert 1991).

Opacity is denoted by κ_λ , and is simply the coefficient of linear absorption of radiation by a medium at a particular wavelength λ . Scattering of radiation is implicitly included in this concept of absorption. That is, opacity is the fractional reduction in a light ray's intensity as it passes through a medium, per unit density of the medium and unit length of the passage. As such, it has units of inverse length multiplied by inverse density, i.e. area per mass (typically cm^2g^{-1}).¹ An equivalent way of describing opacity is as an interaction cross-section or interaction probability per unit mass between the radiation field and the medium, a measure of how opaque the medium is to a given wavelength of light. Consider now a simple non-emitting gas of constant density ρ and opacity κ_λ , also constant for any given wavelength. If a monochromatic light ray of wavelength λ and intensity I_λ passes a distance dr through the gas, the change dI_λ in its intensity will be

$$dI_\lambda = -\kappa_\lambda \rho I_\lambda dr. \quad (2.1)$$

Separating this differential equation and integrating Eq. 2.1 over some path length s along which the intensity drops from I_0 to I , we see that the constant opacity and gas density result in an exponential decrease in intensity with distance, i.e.

$$I = I_0 e^{-\kappa_\lambda \rho s}. \quad (2.2)$$

The characteristic length of this intensity decrease is l , the **mean free path** of a photon. This is the distance over which $1 - e^{-1}$ (i.e. 65%) of photons in the original beam will have been absorbed, and the average distance a photon will travel before it is absorbed. Hence, for our simple gas,

$$l = \frac{1}{\kappa_\lambda \rho}. \quad (2.3)$$

This gives rise to the concept of **optical depth**, denoted by τ . Optical depth is a

¹Occasionally, opacity is defined as an inverse length (cm^{-1}) or a cross-section (cm^2), though cm^2g^{-1} is most common.

dimensionless quantity that describes over how many characteristic length scales of the exponential decrease in Eq. 2.2 a light ray has travelled. Hence, a beam arriving from $\tau = 0$ has been undiminished by its passage, whereas others coming from $\tau = 1$ or $\tau = 2$ have been diminished by factors of e and e^2 respectively, such that for our simple gas

$$I = I_0 e^{-\tau}. \quad (2.4)$$

Generally, areas of gas with $\tau < 1$ to an observer are considered **optically thin** and areas where $\tau > 1$ **optically thick**. The formal definition of optical depth is

$$d\tau_\lambda = -\kappa_\lambda \rho dr, \quad (2.5)$$

which simplifies to give Eq. 2.4 in the case of constant density and opacity.

In reality however, gas in the solar atmosphere has far from constant density or opacity, so the mean free path of photons and the corresponding definition of optical depth will vary with position. This means that the total optical depth to a point will be an integral quantity dependent upon the local opacity and density, themselves strongly dependent upon all the other local properties of the atmosphere via the constitutive relations mentioned in §1.1.1. The preceding example serves to illustrate the concept rather than provide a basis for calculations.

The macroscopic notion of opacity is based upon the microscopic understanding that each gas element will absorb via a range of physically distinct process whose strengths depend upon the energy level transition probabilities of the individual particles in the gas. The probabilities depend upon quantum mechanical properties of the particles and the relative populations of the energy levels. The populations are themselves determined by the locally dominant interaction(s) between particles, which typically show a strong temperature and density dependence. Much more will be said about such statistical considerations in §2.3.2 and §2.3.3. The actual energy levels themselves determine the wavelength dependence of the absorption since photons with wavelengths corresponding to the level difference are being emitted or absorbed. Hence, opacity depends on the local temperature and density of the gas as well as the wavelength of the incident radiation.

In order to deal with the complicated wavelength dependence of opacity, the **Roseland mean opacity** is often introduced. This is a harmonic mean of wavelength-specific opacities, weighted according to the different absorption processes, the quantum mechanical transmission probabilities, the energy level populations and ultimately temperature. The weighting serves to place more emphasis on areas of the spectrum where absorption is lower, as transmitted radiation will tend towards these ‘gaps’ in the opacity spectrum as photons are randomly absorbed and re-emitted. For similar probabilistic reasons, it actually also favours areas where thermal blackbody emission is most dependent on temperature, as a greater increase occurs in emission as photons cross the opacity surface at such frequencies for a given $\frac{dT}{dr}$. If calculated using sufficiently detailed treatment of the emission and absorption processes occurring for a large range of different particles, the Rosseland mean opacity can provide a realistic average opacity of the whole wavelength range for a given temperature, density and chemical composition.

2.2 The Classical Solar Atmosphere

2.2.1 Stratification

The traditional view of the outer regions of the Sun is shown in Fig. 2.1. The **photosphere** is a thin layer where the gas passes from being optically thick to optically thin. The solar ‘surface’ is typically defined as having horizontally-averaged optical depth unity at $5000\text{\AA}$. The location and extension of the photosphere is governed by the highly temperature dependent opacity of the H^- ion (Carrol & Ostlie 1996). The H^- ions provide far more absorption than neutral hydrogen thanks to the presence of their extra electron, and hence are the dominant opacity source. The H^- opacity is fairly constant across wavelength, so where the ion turns rapidly from optically thick to thin we see an approximately blackbody emission spectrum originating from a small layer of gas. Hence, the bulk of the light we observe coming from the Sun originates in this layer, giving rise to the name *photosphere*.

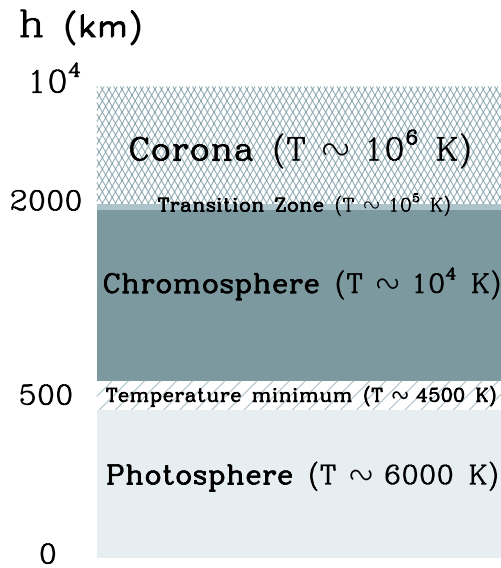


Figure 2.1: The traditional layered picture of the solar atmosphere, indicating the components and their thicknesses. In particular, featuring a $\sim 4500\text{K}$ temperature minimum at the top of the photosphere ($\sim 0.5\text{ Mm}$ above the surface defined as $\tau = 1$). (Figure adapted from Ayres 2002)

The chromosphere is an optically far thinner layer that extends well above the photosphere. It takes its name from the colourful halo seen around the Sun during an eclipse, when the photosphere is obscured and the chromosphere is the dominant light source. Moving upwards in the chromosphere, gas motion becomes less dictated by convection and more by thermal motion and magnetic fields. Above the chromosphere is a small **magnetic transition region** where magnetic fields exert an even greater influence on the diffuse gas than in the chromosphere. Higher still, the **corona** is entirely magnetically dominated and exhibits a range of exotic phenomena like magnetic flux tubes, loops, reconnection events and solar flares. In the upper corona, gas is completely unbound and flows outwards in the solar wind. The convective models and study to be discussed deal with the photosphere and lower chromosphere; regions above this become the realm of coronal simulations mentioned in §1.1.

2.2.2 Temperature, Density and Pressure Structure

As is the case in the solar interior and the convection zone, gas density and pressure in the solar atmosphere drop steadily away from the surface. In the layered paradigm, the temperature structure on the other hand goes through a temperature minimum at

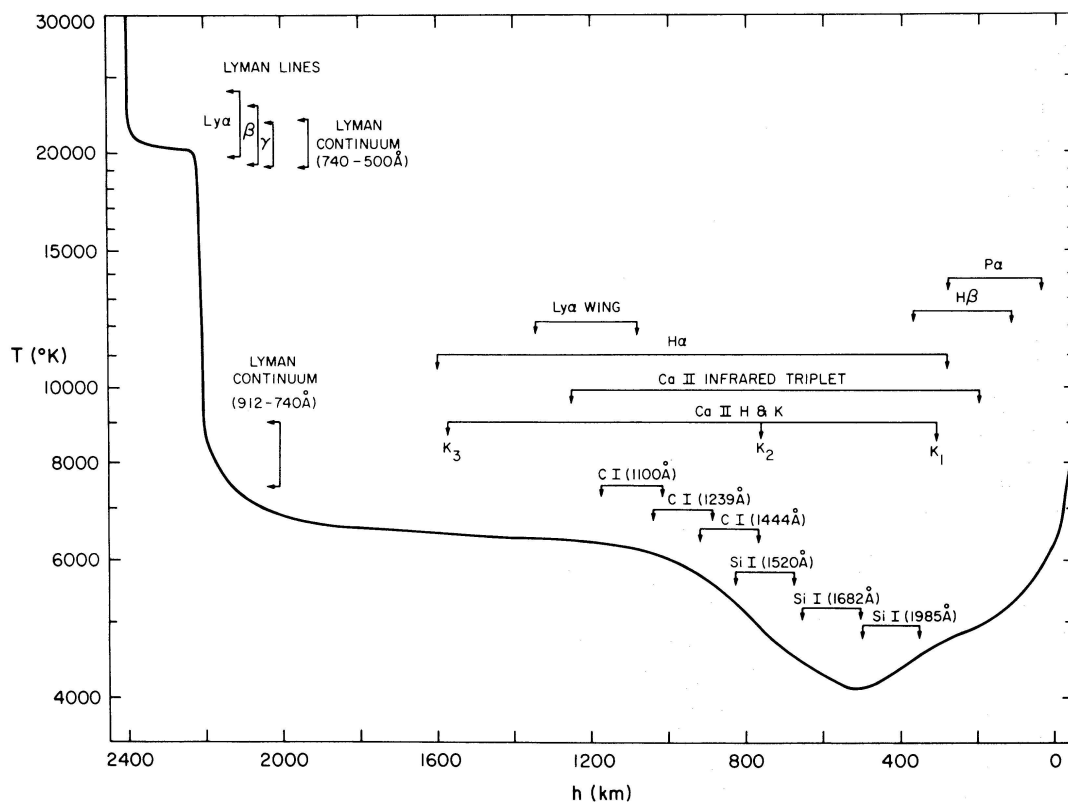


Figure 2.2: The variation of temperature with height in the solar atmosphere according to the traditional layered paradigm. Note the temperature minimum of about 4500K at 500 km, corresponding to the top of the photosphere. Brackets indicate formation regions of various spectral features which agree with this temperature structure. (Figure taken from Vernazza et al. 1973)

about 4500K at the top of the photosphere (Fig. 2.2). Upwards of this minimum, the average temperature rises again through the chromosphere as magnetic and oscillation-driven heating begins to come into effect, before shooting as high as one million degrees in the magnetically dominated corona.

The traditional layered paradigm described and the run of temperature it predicts have recently come under attack (e.g. Carlsson & Stein 1995; Ayres 2002), and there is good reason to believe that the solar atmosphere is not nearly so neatly structured as was once thought. This modern standpoint is linked to the presence of CO, and will be discussed in Chapter 4.

2.3 Spectral Formation

2.3.1 Radiative Transfer

The formation of the solar spectrum is a far more detailed process than can be described in the large scale framework of the Standard Model. Again, the treatment in this subsection draws upon standard texts (Stix 2002; Mihalas 1978; Carrol & Ostlie 1996). In order to determine the intensity of light emitted from the Sun across different wavelengths rather than simply its overall luminosity, an explicit description of the transport of radiation through the gas in the atmosphere must be used. Such a description was in fact provided in Eq. 2.1, though it was an incomplete one. As hinted at towards the end of §2.1, the

gas in the Sun cannot be the non-emitting medium described. Occurring along with the absorption processes encompassed in the variable κ_λ are similarly complicated and microscopically dependent emission processes. Hence, we obtain the proper equation of radiative transfer from Eq. 2.1 via the addition of a **source function** S_λ to the intensity change,

$$\mu dI_\lambda = -\kappa_\lambda \rho I_\lambda dr + \kappa_\lambda \rho S_\lambda dr, \quad (2.6)$$

which becomes

$$\mu \frac{dI_\lambda}{dr} = -\kappa_\lambda \rho (I_\lambda - S_\lambda). \quad (2.7)$$

The variable $\mu = \cos \theta$, where θ is the angle between the path of the radiation and the vertical direction in the Sun has also been introduced here, to account for light rays that do not travel directly upwards before reaching the surface and becoming visible. The factor of $\cos \theta$ is necessary as these rays pass through a greater optical depth than perfectly vertical rays, so experience greater extinction (and more emission processes). Hence, $\mu = 1$ refers to the solar disc centre, and $\mu = 0$ refers to its outermost edge. If we now express Eq. 2.7 in terms of the optical depth as per the definition in Eq. 2.5 we get the **radiative transfer equation** in its standard form:

$$\mu \frac{dI_\lambda}{d\tau} = I_\lambda - S_\lambda. \quad (2.8)$$

The emergent spectrum can then be found by solving for intensity in this differential equation at various wavelengths. The problem of spectral formation then becomes one of establishing opacities and densities, and determining the emissive source function from statistical arguments.

2.3.2 The LTE Approximation

The local thermodynamic equilibrium (**LTE**) assumption is that on a sufficiently small scale, the gas is thought to be in thermodynamic equilibrium (see e.g. Stix 2002). That is, emission and absorption processes occur in equal amounts, and hence no net energy transfer and therefore temperature gradient exist in the gas. The gas particles' energy level populations are hence also static, as every emission is assumed to be immediately matched by an absorption into the same energy level. The populations are determined by collisions between particles only, and therefore follow a Boltzmann distribution. Similarly, ionization levels and velocities are static, following Saha and Maxwellian distributions respectively. As such, a single temperature describes the gas and characterises each of the three distributions. Sounds simple, doesn't it? It is, and is obviously not a situation that can occur over any macroscopic length scale in a stellar atmosphere, as we know that a temperature gradient must exist. On a microscopic (i.e. local) scale however, the assumption of thermodynamic equilibrium can be reasonable in regions of high density and temperature, and serves to make many otherwise computationally prohibitive problems soluble. Typically, LTE is not such a bad approximation for spectral features formed in the lower, denser regions of the photosphere such as the visible continuum and weaker absorption lines², whilst it is not so good a description of higher features such as the ultraviolet

²Line strength is explained in §2.3.5.

continuum or strong spectral lines (Stix 2002). It is certainly not a fair approximation in much of the chromosphere or the corona.

The major consequence of the LTE approximation is that the source function is taken to be simply the well known Planckian black body spectrum i.e. $S_\lambda = B_\lambda$ (Mihalas 1978). This spectrum is a result derived directly from the assumption of a Boltzmann distribution in particle energy levels. The great advantage of this result is that the source function is known as a function of temperature alone. The other great boon of the LTE approach is that having an exact distribution of level populations makes the calculation of opacities a comparatively simple affair. Not too simple mind you; there is still the issue of determining density and temperature at a particular point in the gas before an opacity and source function can be arrived at, but it does make the modelling of the solar atmosphere far more achievable under current computational constraints.

2.3.3 NLTE Calculations

In the cases where LTE breaks down such as in the upper regions of the solar atmosphere, non-LTE (**NLTE**) calculations are necessary to reasonably simulate the observed spectrum. NLTE makes no assumptions as to the distribution of energy level populations or ionization fractions, and explicit calculation of the emission and absorption processes governing them becomes necessary. That is, the assumptions that the levels are populated with a Boltzmann distribution and the ionization follows a Saha distribution are discarded. The assumption that the particle velocity distribution is Maxwellian as in the LTE case is retained however, as the frequency of collisions at photospheric and most chromospheric conditions is still sufficiently high for this to be the case (Stix 2002). Hence, the only place the concept of temperature in an NLTE situation has any meaning is in the velocity distribution of the particles, not the atomic level populations. In the transition region and corona however, even this velocity distribution is not a terribly realistic assumption.

Nevertheless, NLTE situations are generally in a **statistical equilibrium**, where the level populations and ionization rates are still determined by radiative emission and absorption. The equilibrium is a nonlocal one though, where incoming photons from distant regions with different densities and temperatures have a significant effect upon the local level populations and hence emission and absorption rates. In this way, the equilibrium is also non-thermal, as no particular temperature describes the radiation source field. The local effects of spontaneous emission, induced emission, absorption, photoionization, recombination, collisional excitation and collisional de-excitation must hence all be calculated in NLTE (Stix 2002), and also allowed to propagate to distant regions of the gas. As one might imagine, this is a monumental computational task, requiring a multitude of energy level transition calculations to determine the form of the source function. As such, NLTE calculations are not typically employed except over a limited range such as in very high layers, for particular species (both true of Carlsson & Stein 1995, 1997), over very short timescales (Asplund et al. 2004c) and generally in simpler situations such as some of the 1D model atmospheres to be described in §2.4.3.

2.3.4 Chemical Considerations

The discussions in §2.3.2 and §2.3.3 dealt exclusively with the processes of emission and absorption by atoms and their ions. As we observe their spectral signatures, molecules must clearly also be present in the solar atmosphere, and their formation and dissociation are a processes that should be accounted for in any realistic model atmosphere. As the

reader will see in Chapter 4, the formation and break-up of carbon monoxide in particular has a large effect upon atmospheric structure and the emergent spectral lines.

Typically, the molecular number densities are calculated using the approximation of instantaneous chemical equilibrium (**ICE**). ICE assumes that the reagent populations are always given by instantaneous local adjustment to the chemical equilibrium dictated by temperature and density via the Saha equilibrium equations (Uitenbroek 2000a). These are the same set of equilibria used to predict ionization fractions in LTE, based upon Maxwell-Boltzmann statistics which arise from the concept of thermodynamic equilibrium.

Like NLTE calculations, solutions of the non-ICE problem require the simultaneous solution of a large set of rate equations at every point in the gas describing the various processes occurring, which in this case are chemical reactions between all species present. The influence of photodissociation may or may not also be included, though at least in the case of CO its effects are insignificant (Asensio Ramos et al. 2003). Also as with NLTE, the computational cost of non-ICE solutions is very high, and very few applications of non-equilibrium chemistry have been carried out in studies of the solar atmosphere. One very notable exception in the context of the current study is that of Asensio Ramos et al. (2003), and non-ICE has been discussed at times (e.g. Asplund 2004) as well as actively advocated at others (e.g. Uitenbroek 2000a,b). The ICE approximation could overestimate molecule formation and therefore molecular abundance in cool downflowing gas in some cases (Asplund 2004), though at small atmospheric heights where density is high, effects of departures from ICE are sufficiently small to be neglected in most cases. Moving to greater heights and lower densities however, the ICE approximation becomes progressively less accurate.

2.3.5 Line Formation

The fundamental process underlying absorption line formation in a stellar atmosphere is a relatively simple one. The continuum is formed near to where the bulk gas becomes optically thin (roughly speaking, the surface), then has sections of its intensity removed by absorption as it passes through the optically thin gas above. The wavelengths at which sections of the continuum are removed correspond to the gaps between energy levels in the various species present in the gas. Absorption lines in a spectrum therefore change from optically thick to thin at greater heights than the continuum, and the line properties reflect the local physical conditions in the regions where they are formed. Absorption lines therefore provide an invaluable probe of different areas in the atmosphere, as different lines will become optically thin at different heights. The selection of the best set of lines for a particular analysis is a fine art, requiring a very careful evaluation of the transitions in question not only from an atmospheric perspective, but also from observational and quantum mechanical viewpoints.

Emission lines are sometimes also seen, indicating that the gas has become extremely optically thin (i.e. low density) and/or has been heated above the temperature at which the continuum was produced, such that the continuum intensity no longer outshines spontaneous emission from the gas. Emission can also occur due to population inversion, as seen in lasers and masers. Such lines typically issue from non-equilibrium conditions in the chromosphere and corona, and as such (cf. the closing statement of §2.2.1) ‘lines’ in the context of this study should be taken to mean absorption lines unless otherwise stated.

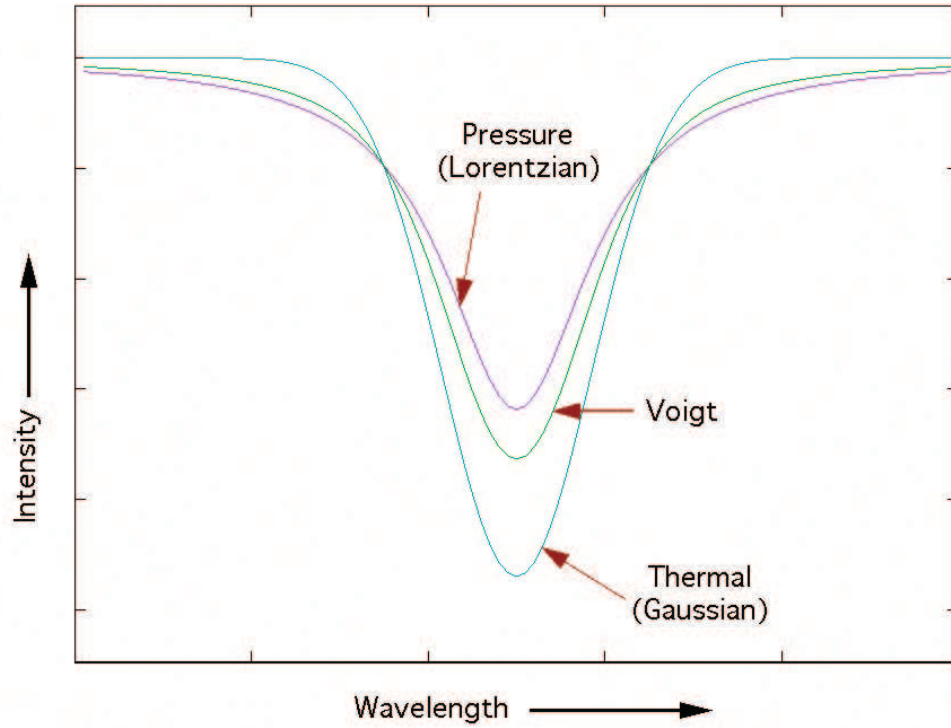


Figure 2.3: Absorption line broadening profiles: Thermal or Doppler (blue), collisional or pressure (purple) and the Voigt profile resulting from the combination of the two (green). Note the way the narrow Gaussian thermal profile dominates in the line core of the resultant Voigt function whereas the diffuse Lorentzian collisional profile dominates in the wings. (Figure is a heavily modified form of a graphic from Christensen 2004)

Line Broadening

Line profiles such as that illustrated in Fig 2.3 always demonstrate some broadening in wavelength. Regardless of any atmospheric considerations, the spectral lines could not be infinitely thin anyway, given the time-energy version of Heisenberg’s uncertainty principle. If the energy levels causing the line were exactly known, the time spent by the atom in each energy state would be completely undeterminable, and the transition could not occur; there is hence some natural spread in energies for all lines under any conditions. In stellar atmospheres, the effects of **Doppler broadening** (or **thermal broadening**) caused by random thermal motion of the gas particles relative to the observer, and **collisional broadening** (sometimes called **pressure broadening**) due to slight shifts in the energy levels caused by electromagnetic interactions during close encounters (‘collisions’) between particles, also become important. Doppler broadening by a species of mass m has a narrow Gaussian characteristic profile of the form

$$\phi_D(\Delta\lambda) = \frac{1}{\sqrt{\pi}\Delta\lambda_D} e^{-(\Delta\lambda/\Delta\lambda_D)^2}, \quad (2.9)$$

where $\Delta\lambda$ is the distance from the line centre of wavelength λ_0 and

$$\Delta\lambda_D = \frac{\lambda_0}{c} \sqrt{\frac{2kT}{m} + \xi_t^2} \quad (2.10)$$

is the Doppler width (half width half maximum) of the Gaussian. The microturbulent velocity ξ_t is an extra ‘fudge factor’ used in analyses based on 1D model atmospheres, introduced to emulate Doppler broadening due to inherently three-dimensional microturbulence in the gas. Without this term, thermal Doppler broadening alone is insufficient in such models to describe the broadening observed in the cores of spectral lines (Stix 2002). Collisional and natural broadening have profiles with broader wings, and as such are together described by the characteristic ‘damping’ Lorentzian profile

$$\phi_C(\Delta\lambda) = \frac{\gamma}{(2\pi\Delta\lambda)^2 + \gamma^2/4} \quad (2.11)$$

where γ is the collisional damping constant. To accurately work out the collisional broadening profile in a stellar atmosphere would be an N-body computational problem of mammoth proportions, as every particle’s approach and collision with every other would have to be explicitly calculated, so even the very best model atmospheres utilise a parameter γ and Eq. 2.11 to describe collisional broadening. These equations were adapted from Stix (2002) and Carrol & Ostlie (1996). Mathematically, the effect of each of these physical effects is to convolve the Dirac delta function of the initially infinitely thin line opacity with each of the profiles (which seeing as convolution is commutative equates to convolving the original delta function with the convolution of the two broadening profiles). The resulting **Voigt profile** can be seen in Fig. 2.3, showing the central domination of the Gaussian thermal profile around the ‘core’ of the line, and the influence of the Lorentzian in its ‘damping wings’. In a calculation of spectral formation, such line broadening considerations are calculated and made part of the relevant line opacities.

Line Properties

The properties of spectral lines tell us about the environment in which they formed. Core wavelength **shifts** generally indicate a bulk upwards or downwards gas Doppler motion (or errors in the laboratory wavelengths!), which can be used to draw inferences about convective motions. Shifts are generally stated in units of relative velocity of the gas that gave rise to them, and in this thesis redshifts are given positive values. Absorption line **depths** indicate the balance between absorption and emission in the core of the line (i.e. where the line becomes optically thin), and are measured in normalised units relative to the continuum. Hence, depths are indicative of temperature and species concentration, which may in turn suggest something about other local thermodynamic quantities.

Line **strength** refers to the area of a spectral line, and is measured in wavelength or wavenumber units of **equivalent width**, equal to the width of a rectangle under the continuum of the same area as the line. Typical units for stating equivalent width values are milliÅngströms (mÅ) or milliKayser (mK), where a Kayser is a wavenumber unit of inverse centimetres (cm⁻¹) occasionally used in the infrared. The strength of a line generally gives an indication of how deep in the atmosphere it has formed, as lines forming closer to the continuum will show less absorption because more of the thermal emission which produces the continuum is occurring around and above them. This serves to ‘wash out’ their spectral features in comparison to those forming further away from the

continuum, where the continuum optical depth $\ll 1$ and the lines are hence much stronger (Carrol & Ostlie 1996). Line cores are therefore formed higher in the atmosphere than wings, with the curve of a spectral line reflecting absorption occurring in a continuous way at all heights between those of core and continuum formation. The concepts of shift, depth and strength of an absorption line are shown diagrammatically in Fig. 2.4.

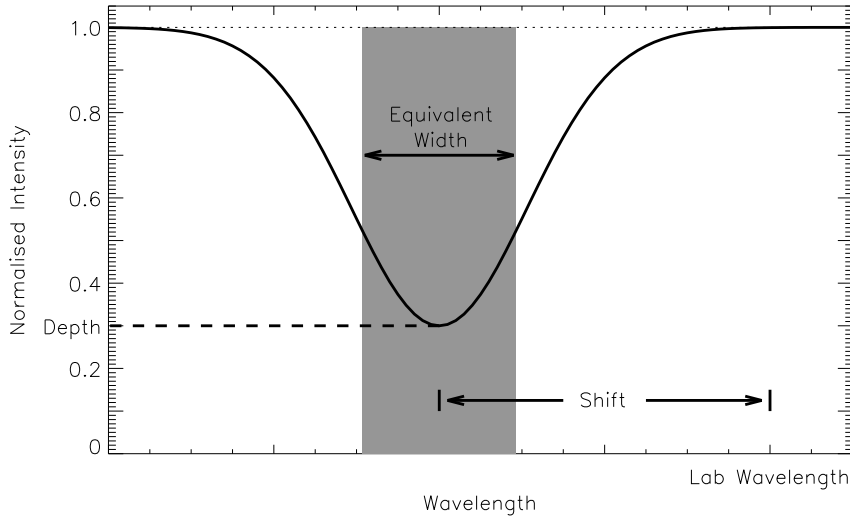


Figure 2.4: Illustration of spectral line strength, depth and shift. The shaded rectangle defining equivalent width has the same area as that between the curve and the dotted continuum line.

Of special significance to this study are the line **bisectors**. A line bisector is the single line vertically bisecting an absorption profile, running from its deepest intensity point at the core to the continuum in such a way that it is equidistant in wavelength from each side of the profile at all points along its length. When considering a spectral line, it must be realised that the observed spectrum is averaged in both space and time. At different positions across the solar surface and at different points in time, radiation emerging from the core of a spectral line may exhibit a different red or blue shift corresponding to the velocity of the particular fluid element from which it was emitted. When observing an overall solar spectrum, these spatially distinct profiles, each with their own shifts, sum to produce the average spectrum. Hence, the shape of absorption profiles can be used to determine to what extent particular lines form in upflows, downflows or horizontally moving gas. The bisectors of the lines are what betray this information to us, providing a measure of a line's asymmetry. The summation of profiles formed in regions with different velocity structures is demonstrated in Fig 2.5, along with the bisectors arising from each. Bisectors slanted bluewards ($\backslash$) arise from a dispersion of upwards velocities from the core, those slanted redwards ($/$) arise from a dispersion of downwards velocities. Combinations of upwards and downwards velocities produce $\subset$ or $\supset$ shapes depending upon the relative strengths of the different components. Static profiles, as produced by 1D hydrostatic model atmospheres due to their lack of time-dependence and therefore velocities, result in vertical bisectors ($|$). These relations are indicated also in Asplund et al. (2000b) and Gray (1992).

It should be noted that the shapes of the bisectors are about the line core, so the velocity indication they give is only relative to the motion of the core-formation region. If the velocity shift of the entire line (and bisector therefore) is well beyond any variation

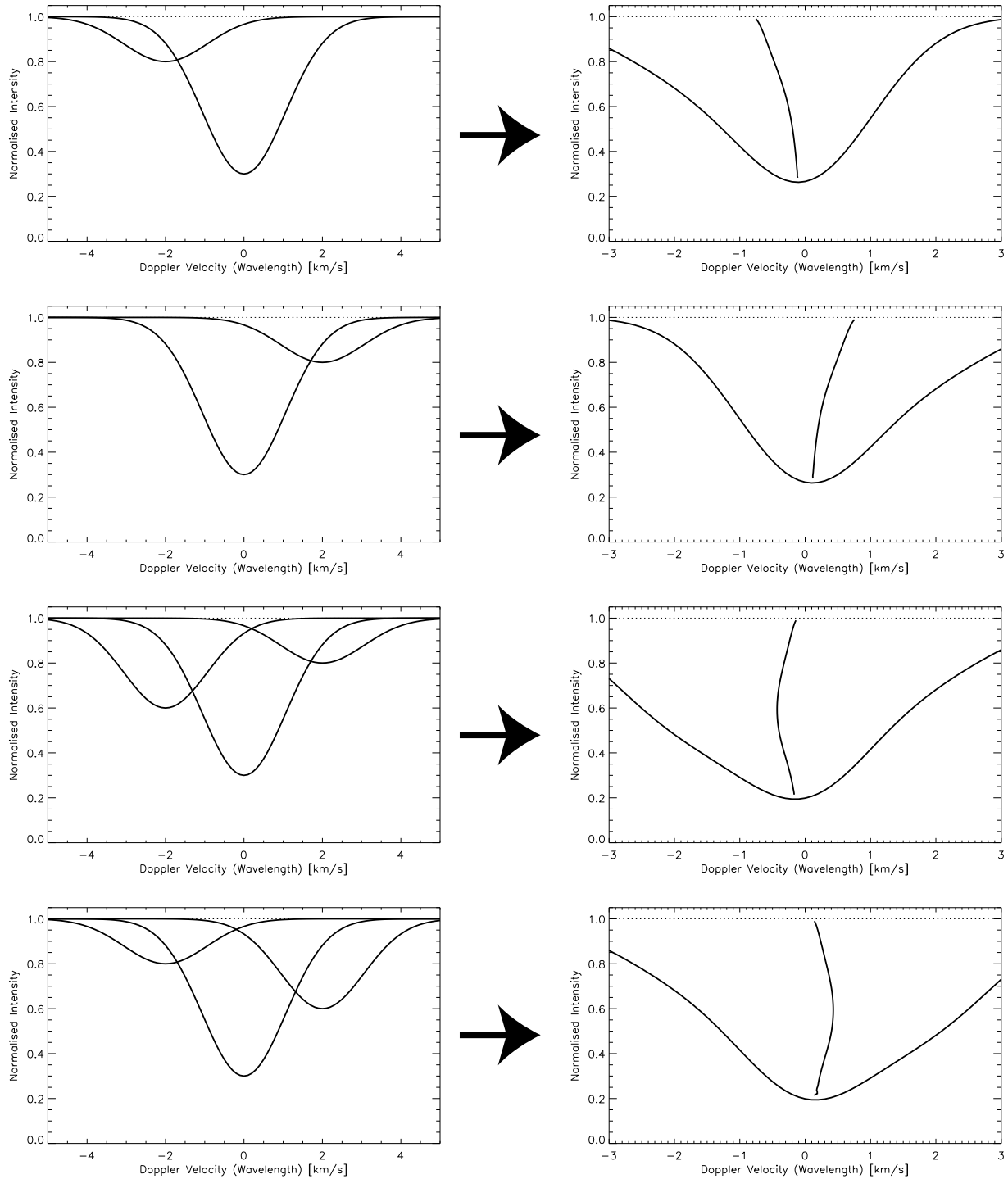


Figure 2.5: Example velocity dispersions and the bisectors resulting from them. *Top:* Strong component, produced high in the atmosphere where velocities are predominantly horizontal, and weaker blueshifted component produced lower and in upflowing granules. *Upper Centre:* Strong unshifted component and weaker redshifted component due to downflowing intergranular lanes. *Third:* Strong core component with both upflow and downflow components, where the component associated with upflowing granules is stronger than that of the downflowing intergranular lanes. This is the most common configuration in the solar atmosphere. *Bottom:* As previous, but with the intergranular component stronger than the granular. Not shown is the fact that in 1D hydrostatic models, bisectors produced are always perfectly vertical since velocity fields are not permitted by such models.

due to bisector shape, the shape will be indicative only of the distribution of velocities about the bulk velocity indicated by the core shift. However, laboratory wavelengths for the transitions considered and the observational wavelength calibration are often not sufficiently accurate for the determination of bisectors on an absolute velocity scale. For this reason, bisectors are commonly artificially shifted to have their feet (i.e. the line cores) at zero velocity relative to the observer (e.g. Blomme et al. 1994). This is very often the position of solar bisectors anyway without such zeroing (Gray 1992), at least for strong lines, as the deepest parts of a line typically form at the top of the convective granules where the gas velocity is predominantly horizontal. Nowadays though, better solar observations and higher precision measurements of the solar rotation generally mean for the Sun, bisectors can in fact be determined on an absolute scale (e.g. Asplund et al. 2000b).

2.4 Convection

At the simplest level, convection is instability against spatial perturbation up or down a density gradient. That is, if gas in the convective zone is somehow perturbed upwards or downwards, it will continue in that direction until it is heated or cooled sufficiently to send it back the other way. As such, convection involves the ‘turning over’ of the outer third of the solar atmosphere. The derivation typically performed in standard texts (e.g. Kippenhahn & Weigert 1991; Stix 2002) of the basic condition for convective instability involves a gas element of density ρ at a height r perturbed to a new height $r + dr$ where the ambient density is ρ_0 . The gas element is assumed to expand sufficiently quickly that the process occurs adiabatically, but sufficiently slowly that the new pressures inside and outside the element balance. This assumption is justified on the basis that in stellar atmospheres the sound-crossing time of an element is significantly smaller than the energy exchange timescale between it and the environment (Stix 2002). If the new density of the gas element is greater than the outlying density for upwards perturbations or less for downwards ones, the element will obviously return to its starting point and the atmosphere will be stable at r . The difference between the new density ρ^* in the element and the ambient density will hence be given by

$$\rho^* - \rho_0 = dr \left[\left(\frac{d\rho}{dr} \right)_a - \frac{d\rho}{dr} \right], \quad (2.12)$$

where the subscript a denotes the adiabatic density gradient. Assuming the gas to be ideal, i.e. $P = \rho kT/m$ where m is the mean gas particle mass, this is

$$\rho^* - \rho_0 = dr \frac{Pm}{kT^2} \left[\frac{dT}{dr} - \left(\frac{dT}{dr} \right)_a \right]. \quad (2.13)$$

In the case of instability to the perturbation, where if $dr > 0$ then $\rho^* < \rho_0$ or vice versa, we now have the **Schwarzschild criterion** for convective instability

$$\frac{dT}{dr} < \left(\frac{dT}{dr} \right)_a \quad (2.14)$$

The variation of mean particle mass has been ignored here for simplicity, but the result would have been identical was it not. Hence, for convection to occur, given that temperature essentially decreases outwards ($\frac{dT}{dr} < 0$), the temperature gradient must be steeper

than its adiabatic value.

2.4.1 Mixing Length and Turbulence

The traditional method of treating convection in the solar atmosphere is to appeal to mixing length theory (**MLT**) and its freely adjustable parameter α . This parameter describes the ratio of the convective **mixing length** to the **pressure scale height**. The pressure scale height describes the typical scale length over which pressure changes in the convective atmosphere, in much the same way l does the change of radiation intensity. Like the mean free path in the context of the solar atmosphere, the pressure scale height is a gross approximation of the truth, giving a rough indication only of pressure variation. The same is true of the mixing length, which is supposed to indicate the average ‘length of travel’ of a convective gas element, before it dissolves into the surrounding gas and deposits the energy excess or deficiency it has carried from another region. This is a doubly poor explanation, as the convective gas does not travel a distance and then disappear, but overturns constantly throughout the convection zone whilst absorbing and emitting energy. Nevertheless, mixing length is a useful approximation, as in the 1D case it makes the estimation of energies transported by convection and the associated overall superadiabatic temperature gradient possible. This is done via the solution of a series of algebraic equations relating the adiabatic, radiative (if convection were suppressed) and pure convective temperature gradients (Mihalas 1978), allowing at least some sort of simulation of convection in 1D model atmospheres rather than none.

Further gas motions not described by 1D models (even with MLT) are necessary to produce profiles sufficiently broadened to resemble observed lines. For this reason, two more freely adjustable parameters are introduced: The microturbulence ξ_t described in §2.3.5 and a macroturbulence V_{mac} . By representing turbulent motion on two different length scales, these terms are supposed to account for any gas motions not otherwise included in a 1D model with MLT treatment. The macroturbulent velocity is used to describe non-local turbulence in a similar way to the microturbulence describes local turbulence (Gray 1992; Stix 2002). That is, V_{mac} is the half width half maximum of a convolving Gaussian applied to broaden an entire line profile rather than just the opacity core, as is the case with ξ_t .

2.4.2 The Equation of State

Although the constitutive relations described in §1.1.1 are sometimes collectively known as the ‘equations of state’, it is most common to see the constitutive relation for density (expressed as a function of pressure, temperature and composition) rearranged with P as the subject and referred to as the **pressure equation of state** or simply the **equation of state**. The simplest equation of state is just the ideal gas law $P = \rho \mathcal{R}T/\mu$, though in less dense areas towards the top of the convection zone radiation pressure $P = aT^4/3$ must also be included, where a is proportional to the typical particle cross section for radiative collisions. As with just about everything else in stellar atmospheres, these in turn depend upon the number of particles of different species and ionization states. Hence, the equation of state depends upon accurately describing the ionization states of all the species in the gas, which is easily achieved in LTE via the Saha equations, but not very easily in NLTE.

Most importantly, a good equation of state will include a suite of electrostatic, degenerative and assorted other non-collisional pressure correction terms (Stix 2002; Hummer & Mihalas 1988). The most rigorous derivation of an appropriate equation

of state for a given situation is to follow the procedure of free-energy minimisation (Hummer & Mihalas 1988; Mihalas et al. 1988; Stix 2002) fundamental to statistical mechanics. Typically, pressures are calculated across a grid of representative densities and temperatures using an appropriate equation of state, stored and interpolated between when required by model atmosphere simulations. The same procedure is performed for opacities; this serves to save computational time that would otherwise have been spent explicitly calculating pressures and opacities for every density and temperature combination.

2.4.3 1D Models of the Solar Atmosphere

A large number of one-dimensional solar atmospheres have been produced, each containing slightly different treatments of the topics discussed so far. Those that will be discussed are the Holweger & Müller (1974) (HM) and MARCS (Gustafsson et al. 1975) model atmospheres, which both assume LTE. The former because of its longevity; the HM model seems from its overwhelming use in the literature to have been the only one to stand self-consistently without improvement over the years, regularly returning abundance measurements (e.g. Harris et al. 1987; Asplund et al. 2004c; Grevesse et al. 1984) showing little wavelength, strength or excitation potential dependence (cf. Chapter 5). The latter is considered because of its updated opacities (Asplund et al. 1997), producing less scatter in abundance measures and almost as little wavelength, strength and excitation dependence as the HM model (e.g. Asplund et al. 2004c). In short, HM is the proven practitioner in 1D models, but everyone has their own preferred second opinion; ours is MARCS.

The HM model was designed initially for the analysis of solar barium lines, and is based upon a completely empirical choice of temperatures and correspondingly calculated pressures across 29 optical depths ranging from 10 to 10^{-7} . The MARCS model atmosphere began life as a grid of possible model atmospheres for giant stars before being recomputed with solar element abundances, and the effects of line blanketing (continuum darkening by multiple absorption lines) included (Asplund et al. 1997). Improved line opacities were also included, provided by Kurucz (1993).

The MARCS model atmosphere is a more physically satisfying model than the HM, as it derives its temperature and pressure structure from a realistic series of opacities and an equation of state for pressure rather than arbitrarily choosing the structure to fit observations. This also allows it to be calculated over any desired resolution rather than simply interpolated to the required resolution as the HM model must. As 1D models, both require the use of appropriate micro and macroturbulences for agreement with observation. The temperature structures of the two models are shown in Fig. 2.6, along with the average temperature structure of the three-dimensional simulations to be described in Chapter 3 for comparison. It can be seen that the MARCS model better resembles the average 3D structure than the HM model, supporting the idea of its improved realism (in so far as 1D models can be considered realistic).

Various NLTE 1D models exist (e.g. Vernazza et al. 1981; Carlsson & Stein 1995, 1997), as the computational demands of NLTE can often be partially realistically met in 1D, unlike the 3D case. Though often limited in their application to specific lines (CO vibration-rotation in the case of Uitenbroek (2000b) and hydrogen and singly ionized calcium in the case of Carlsson & Stein), such models can add significantly to our understanding of atmospheric processes (as will be detailed for these two studies in Chapter 4). As discarding the LTE assumption is inherently more realistic, such models are

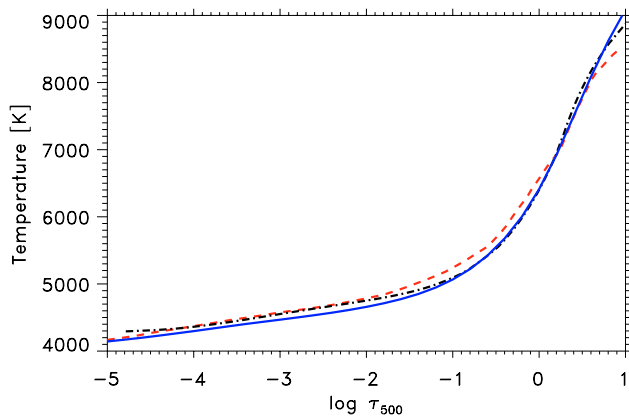


Figure 2.6: Temperature structures of MARCS (black), HM (red) and 3D (blue) model atmospheres. Note the closer agreement between MARCS and the 3D case than between HM and 3D, interpreted as an indication of the greater realism of MARCS over HM. (Figure taken from Asplund et al. 2004c)

certainly an improvement in their own narrow zones of applicability over HM and MARCS, and as such represent an important parallel frontier to 3D models in the field of stellar atmospheres.

2.4.4 Fundamentally Different Approaches to Atmospheric Modelling

The HM model is a **semiempirical** one: its temperature structure was entirely manufactured to fit the observed solar spectrum as best the authors could manage. Most 1D atmospheres employed today as alternatives to the HM model are what are known as **theoretical models**. These models, like MARCS and some of those employed by Uitenbroek (2000b), allow the temperature and pressure (or equivalently, density) structure to be determined from some basic solar input data such as gravity, effective temperature and composition. They are based upon the concept of mixing length and as such contain freely adjustable parameters α , ξ_t and V_{mac} , making their tuning an empirical affair but their overall derivation somewhat less so than models such as the HM one.

Ab initio atmospheric models on the other hand begin with the fundamental physics contained in the conservation equations of fluid dynamics, solving these in a self-consistent way as an alternative to the mixing length approach. As such, the free parameter α is not required. The models constructed by Carlsson & Stein (1995, 1997) were of this ilk, though still one-dimensional and unable to realistically describe turbulence (being structurally unique to the dimension in which it occurs and actually impossible in 1D), therefore still requiring V_{mac} and ξ_t . The three modelling approaches described quite plainly increase in order of explanation, in their realism in describing the physics of the solar atmosphere. If we accept the fundamental philosophical interpretation of physics as describing reality, then the ab initio models clearly have more to say of significance than the others. The 3D models to be described in the next chapter are squarely in this camp, making away with even the turbulence parameters.

3D Hydrodynamical Model Atmospheres

Like any large-scale computational undertaking, fully three-dimensional simulations of convection have been developed over a period of many years. In the early stages, they provided a mechanism for the qualitative investigation of the topology of convection (Stein & Nordlund 1989) and solar oscillations (Stein et al. 1988). They have since grown in sophistication and resolution, fuelled by a parallel increase in computational power, and the default incarnation today is that laid down in Stein & Nordlund (1998). Whilst the version of the hydrodynamical models to be described in this chapter and predominantly utilised in the study is essentially the Stein-Nordlund one with some alterations, an improved version of the same code (Trampedach 2004) does enter the analysis in §7.3.

Throughout the previous chapter, the astute reader may have sensed an emerging dichotomy between the convective and spectral formation sections of the atmospheric theory. This is no coincidence, as properly detailed, spectral formation radiative transfer calculations are typically only performed after the atmospheric structure has been determined from convective considerations. This does not mean that model atmospheres don't contain radiative transfer adjustments to the internal energy of the gas, just that to perform them in as much detail as is required for analysing line properties across the spectrum is not computationally feasible. Instead, such calculations are often performed on a per-line basis after the fact. As such, the two calculations can be independently performed in LTE or NLTE, though the studies thus far described have only performed both in the same manner. The 3D models of this chapter are entirely LTE, except for some special cases briefly discussed in §3.4. This chapter is correspondingly split into discussions of the convective (§3.1) and radiative transfer (§3.2) parts of the 3D simulations, followed by a review of general (§3.3) and specific (§3.4) past results.

3.1 Hydrodynamics

The simulation of convective motion is achieved by solving the 3 fundamental equations of fluid mechanics, expressed in the form

$$\frac{\partial \ln \rho}{\partial t} = -\mathbf{u} \cdot \nabla \ln \rho - \nabla \cdot \mathbf{u}, \quad (3.1)$$

$$\frac{\partial \mathbf{u}}{\partial t} = -\mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{g} - \frac{P}{\rho} \nabla \ln P + \nabla \cdot \sigma, \quad (3.2)$$

$$\frac{\partial e}{\partial t} = -\mathbf{u} \cdot \nabla e - \frac{P}{\rho} \nabla \cdot \mathbf{u} + Q_{rad} + Q_{visc}, \quad (3.3)$$

(Stein & Nordlund 1989, 1998, with correction of a misprinted “ p ” in the left hand side of Eq. 3.1 in the 1998 paper to “ ρ ”, following consultation with Mihalas & Weibel-Mihalas 1999). Eq. 3.1 is the equation of continuity or mass conservation and Eq. 3.2 and Eq. 3.3 are the momentum and energy conservation equations respectively. The vector $\mathbf{u}$ is the velocity field, $\mathbf{g}$ the gravitational force vector and σ the viscous stress tensor. Q_{visc} is the viscous energy dissipation, whilst Q_{rad} is the radiative energy term found by the solution of the transfer Eq. 2.7, integrated over all wavelengths and a given solid angle Ω of radiative propagation

$$Q_{rad} = \int_{\lambda} \int_{\Omega} \kappa_{\lambda} \rho (I_{\lambda} - S_{\lambda}) d\Omega d\lambda, \quad (3.4)$$

where the expression from Stein & Nordlund (1998) has again been altered, this time with κ_{λ} (in units of cm^2 rather than cm^2g^{-1}) replaced by $\kappa_{\lambda}\rho$ in order to be consistent with notation in §2.3.1 and following consultation with Mihalas & Weibel-Mihalas (1999).

3.1.1 Realistic Equation of State and Opacities

The pressure term in Eq. 3.1-3.3 must come of the equation of state, as described in §2.4.2. There pressure was discussed as a function of density and temperature, though here the equation of state must be in terms of density and energy. This is an equivalent formalism; any thermodynamic quantity can be determined from any two others (Mihalas & Weibel-Mihalas 1999), so moving between the two given a known equation of state is straightforward.

Stein & Nordlund (1998) utilise the equation of state and associated opacities contained in the Uppsala stellar atmospheres package (Gustafsson et al. 1975, and updates described in §2.4.3) that sired MARCS. A more modern and rigorously derived equation of state is that of Mihalas, Hummer and Däppen (Hummer & Mihalas 1988; Mihalas et al. 1988), known as the **MHD** equation of state (not to be confused with the magnetohydrodynamic version of Eq. 3.1-3.3). This equation of state package contains a broader range of physics than the Uppsala package, including external and internal particle free energies, electron degeneracy and electrostatic interactions. For this reason, and in contrast with the Stein & Nordlund (1998) version, the model used in this study makes use of the MHD equation of state for hydrodynamical calculations. One notable deficiency of the MHD equation of state however is that it does not deal with molecules, whereas the Uppsala equation of state does. Whilst this is important in the final production of a simulated spectrum if dealing with molecular lines (cf. §3.2), the greater physical realism of the MHD equation of state outweighs its molecular shortcomings in the realm of the hydrodynamical simulations, where individual atomic or molecular partial pressures are less crucial. Opacities, including those of molecules, are still derived via the Uppsala package in the current study. As was described in §2.4.2, pressure and opacity values are tabulated and interpolated between.

3.1.2 The Method of Solution

Eq. 3.1-3.3 are solved numerically, using a third order leapfrog time advance with spatial derivatives from third order splines (cf. Press et al. 2002). A consequence of the leapfrog

time advance technique is an emergent decoupling in the simulation of adjacent points in time and space (Press et al. 2002), which is stabilised in the model atmosphere code by use of a **numerical viscosity**. This viscosity is included in the code to prevent ringing, short wavelength noise and associated numerical artefacts that arise from the leapfrog scheme. It is a purely numerical device introduced for stability, not a physical quantity, and as such *does not* constitute a freely adjustable parameter.

Eq. 3.4 is solved simultaneously with the hydrodynamic equations using the Feautrier method (cf. Mihalas 1978; Mihalas & Weibel-Mihalas 1999). The equation was made three-dimensional through the introduction of solid angle, and the integration over it is achieved by the solution of one-dimensional radiative transfer along a series of variously inclined rays, as well as the vertical itself. That is, the integral over Ω in Eq. 3.4 becomes a sum over these representative rays within the solid angle. Similarly, line blanketing is taken into account in a computationally achievable way via the use of **opacity binning** (cf. Nordlund 1982). This method involves the sorting of monochromatic opacities into groups of similar value (‘binning’), and the average within each group taken to be the opacity for that bin. Each bin is then given a weighting in the final analysis according to how many wavelength points it contains. Hence, the integral over λ in Eq. 3.4 becomes a sum over all bins, a far more computationally tractable prospect.

3.1.3 Extent and Boundary Conditions

Owing to its size, there is no way even modern computers could hope to realistically model the entire convection zone of the Sun. Instead, only the upper layers (owing to their relevance to the observed spectrum and granulation pattern) of the convective zone are simulated. The Stein & Nordlund (1998) model extends downwards over 3 Mm from 0.5 Mm above the surface, whilst our implementation covers 3.8 Mm with just less than 1 Mm above the solar surface. Both versions have 6 Mm extents in each horizontal direction. These dimensions allow room for the presence of at least 10 granules on average, and reach low enough for the gas at the bottom of the domain to be “nearly adiabatic” (Asplund et al. 2004c).

Due to this finite domain of simulation, appropriate boundary conditions are necessary. The horizontal boundaries are made periodic, as the assumption that the full atmosphere essentially consists of identical domains tiled horizontally is implicit in the choice of a finite horizontal extent. That is, incoming and outgoing gas at one horizontal boundary is matched by outgoing or incoming gas with the same thermal properties at the opposite boundary. The lower boundary allows transmission but is conservative of mass by the adjustment of incoming gas pressure. Outflowing entropy is also matched by the adjustment of inflowing density and internal energy.

The open upper boundary is an extended upper layer of the simulation, such that conditions are imposed across and at the top of it, but the simulation is not considered valid above the bottom of the layer. This layer provides a means to deal with the unknown properties of infalling gas from above the domain, where magnetic fields not entering the simulations likely play a large role. This is achieved by application of hydrostatic density and zero velocity gradients across the layer. Across the uppermost boundary, a single space-averaged internal gas energy calculated from the previous layer is imposed upon both incoming and outgoing gas. In this way, gas is let into the simulation from the top of the boundary layer and relaxes under the influence of its surroundings, approximately equilibrating to the conditions of the simulation by the time it reaches the next layer.

In addition, Stein & Nordlund (1998) held the energy at the upper boundary constant in time as well as space; we do not, allowing temporal energy fluctuations in the incoming and outgoing gas.

3.1.4 Resolution

The primary simulation employed in this study was performed on an xyz cartesian mesh of $200 \times 200 \times 82$ points; that described in Stein & Nordlund (1998) was on one of $125 \times 125 \times 163$ points. Asplund et al. (2000a) demonstrated that a resolution of even $100 \times 100 \times 82$ across the stated domain is sufficient to properly model convection in the Sun, with convergence achieved in the characterisation of line profiles, shifts and asymmetries, as well as abundance measures. At grid sizes below this, resolution error was apparent, but more detailed grids brought little improvement over the $100 \times 100 \times 82$ case. To therefore be absolutely confident that no resolutional effects enter our analysis, we choose to work with 200 points in each horizontal direction.

3.2 Radiative Transfer and Line Formation in 3D

Having generated a model solar atmosphere in the manner detailed in the previous section, the task remains to reproduce with it a section of the solar spectrum. To this end, before detailed radiative transfer calculations are carried out on the now established convective structure, the atmosphere is interpolated to a lower resolution grid with a reduced depth extension. This makes the computational time for spectral synthesis reasonable and has virtually no deleterious effect upon the spectrum produced (Asplund et al. 2000a). The interpolation produces a $50 \times 50 \times 82$ grid with the same horizontal dimensions as its parent and a vertical scale extending approximately 0.7 Mm below and a little less than 1 Mm above the solar surface. This reflects the fact that nearly none of the radiation emitted from the lower areas of the hydrodynamical simulation domain contributes to the emergent spectrum, owing to the local optical depth.

The three-dimensional radiative transfer equation (Eq. 3.4) is explicitly solved across the entire interpolated domain for a given line, and a resultant spectrum produced for each point in the horizontal grid. This is typically performed individually for 100 snapshots saved from the hydrodynamical simulation, spanning roughly an hour of real solar time. Profiles are then spatially and temporally averaged, and integrated over the entire solar disc if required, assuming the Sun’s rotational velocity of 1.8 kms^{-1} (Asplund et al. 2004c).

The solid angle integration in each radiative transfer calculation takes the form of a sum of 17 differently oriented light rays. Unlike the hydrodynamical case, opacity binning is not required, and the monochromatic line opacity is explicitly used for the calculation, determined along with the continuum opacity from the Uppsala stellar atmospheres package. Because it does not consider molecules, the MHD equation of state is used only in the case of atomic line formation, whereas the Uppsala equation of state under the assumption of ICE is used for simulation of molecular lines. In this study, seeing as CO lines are to be investigated, the Uppsala equation of state will be used exclusively for line formation calculations.

3.3 General Properties of 3D Solar Simulations

Stein & Nordlund (1989, 1998) provide a thorough description of the general properties

of the simulations. Seeing as the model presented was by this time fully developed, the later paper as such represents *the* definitive exposition of the general process of solar convection¹; what follows is a summary of this work.

3.3.1 Granulation and Flow Structure

The emergent granulation pattern produced by the simulations is shown alongside an actual photograph of the solar surface in Fig. 3.1. Following corrections to the theoretical image for instrumental and seeing effects, the agreement is striking. Note the similarity in granular size, brightness and contrast. The corresponding surface of optical depth unity is shown in Fig. 3.2. As expected, this surface is highly corrugated, reflecting the variation of opacity and density with thermodynamic inhomogeneity across the domain. In particular, the surface of Fig. 3.2 is shaded according to gas temperature, demonstrating the rapid increase in H^- opacity with temperature.

Convective flows of the gas are illustrated in Fig. 3.3. Hot gas flows gently upwards in the granules before rapidly cooling as it becomes optically thin, decreasing in buoyancy and changing direction to flow almost horizontally away from the granule centres. At the boundary between granules, dark, cool intergranular lanes form where the horizontally moving gas meets and flows downwards. The downflowing gas moves somewhat horizontally also, and multiple intergranular lanes merge beneath the surface to produce a steadily increasing granular scale with depth. Most upflowing gas is not sufficiently close to the centre of a granule to ever reach the surface, being pushed horizontally well before it can and then downwards again. Typically, all downflowing gas will be reheated and recirculated eventually.

Very high above the surface, at low optical depths, the brightness contrast seen in Fig. 3.1 between granules and lanes actually reverses. This is because gas that has made its way this high has actually ‘overshot’ into convectively stable regions and therefore cools much more than its surroundings before dropping again, producing a network of bright lanes and dark granules.

Granules push out against each other, increasing or decreasing in area over the course of the simulation. If a granule becomes too large, the gas upwelling from its centremost regions cools so much before reaching the intergranular lanes that it locally overcomes the upflow and begins to form its own downflow, fragmenting the granule. This is facilitated by the increase in gas density and pressure over a granule centre as upwelling gas cools progressively more, in turn steadily reducing the velocity of upflowing gas in the region until a downflow begins. Reduction in temperature over granule centres can be seen if one looks closely at the area above the large granule in Fig. 3.3. In these two ways, the granular pattern can be seen to evolve over the course of the simulation, in the same way we observe the Sun’s surface to. The decreased central flow velocity in granules due to pressure build-up can also be seen to cause edge-brightening (evident in Figs. 3.1 and 3.4) as energy transport is inhibited over granule centres.

As can be seen in Fig. 3.1, the granules account for the bulk of the area of the solar surface. Because of this, line formation is dominated by absorption in granules, so line cores generally show a convective blueshift and spatially averaged bisectors are dominated by the velocity structure within granules rather than lanes. Hence, weaker lines forming

¹Whilst later models could and likely will be more physically correct by being NLTE, including magnetic fields or whatever, the *general* properties of the convective structure should be unchanged by such fine adjustments.

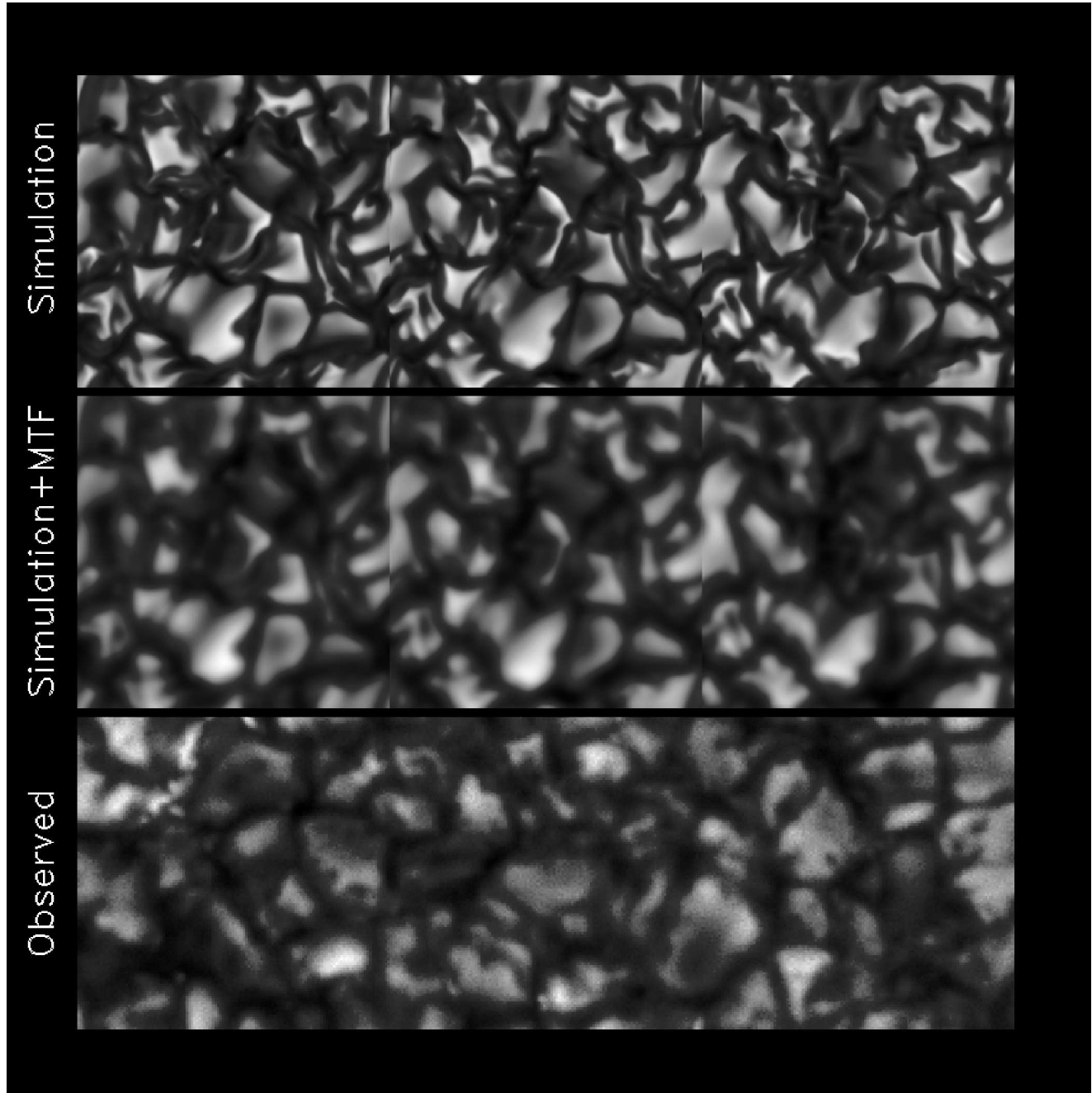


Figure 3.1: Comparison of granulation patterns produced by convective simulations (top two rows) and observed with the Swedish Vacuum Telescope, La Palma (bottom row). The upper row shows the raw emergent intensity, whereas the middle row of images have been convolved with Airy and point-spread functions to simulate seeing and instrumental effects (middle). Individual simulated images are the full 6×6 Mm at 1 minute intervals, the observed image is a region measuring 18×6 Mm. (Figure taken from Stein & Nordlund 1998)

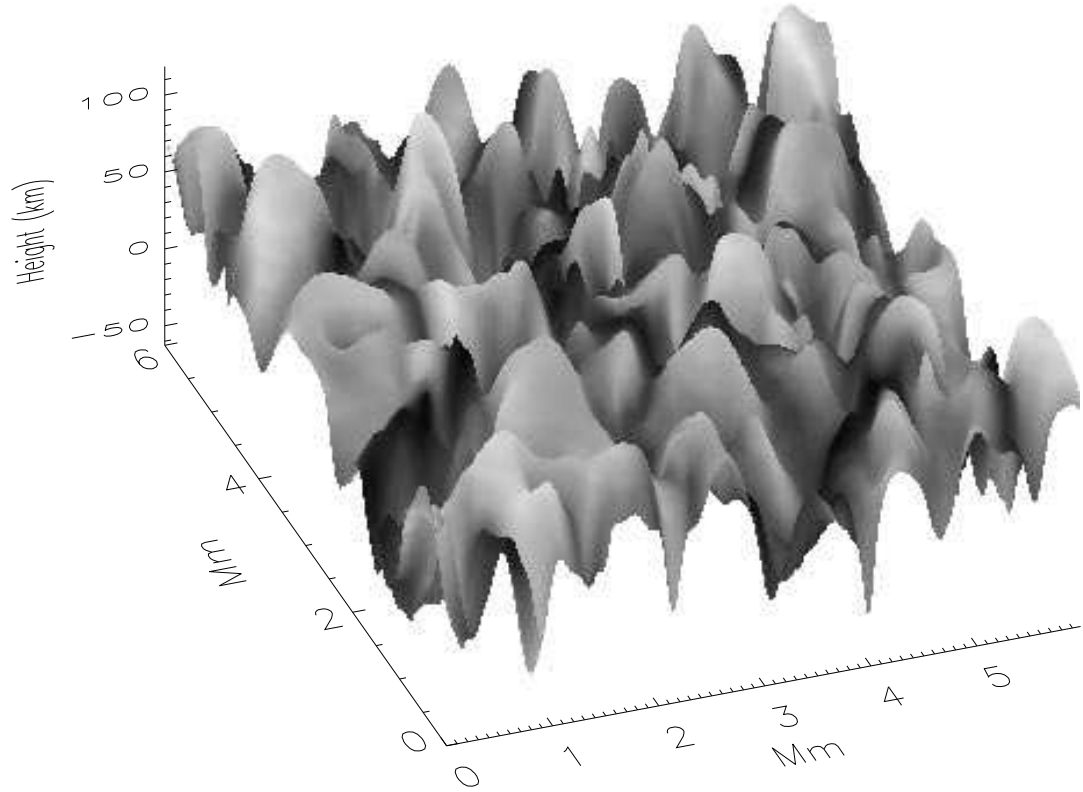


Figure 3.2: Corrugated surface of unit optical depth in 3D convective simulations, shaded according to gas density. Note that cooler gas reaches unit optical depth lower than warmer gas, reflecting the sharp temperature dependence of the H^- opacity. (Figure taken from Stein & Nordlund 1998)

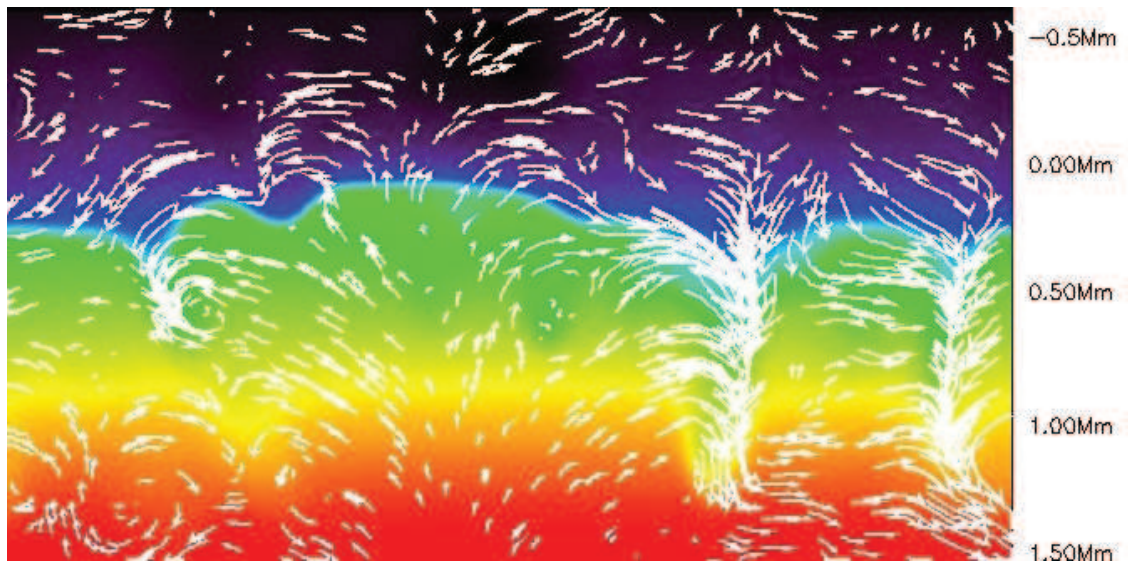


Figure 3.3: Convective velocity field across a single vertical slice through the simulation, shaded according to temperature; warmer colours indicate hotter gas. Note the circulatory motion of the gas and the differentiation into granules and intergranular lanes. Note also the slight temperature reduction over the large granule; this gives rise to contrast inversion at such heights and contributes to granular evolution. (Figure obtained from Asplund 2004)

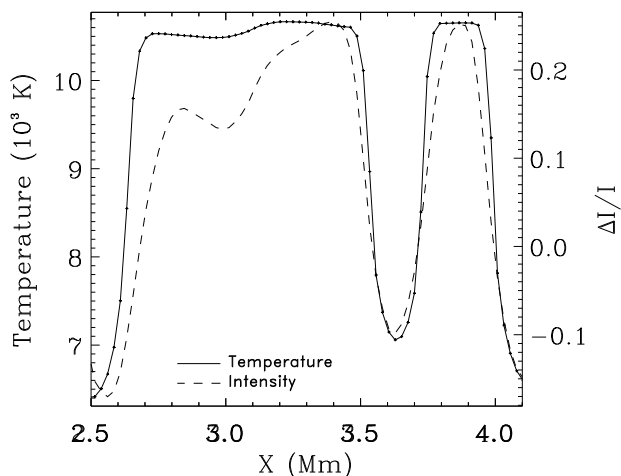
low in the atmosphere will exhibit most absorption at heights where blueshift velocities are large, but less at lower velocities, resulting in $\wedge$ -shaped bisectors. Likewise, strong lines formed very high in the atmosphere will exhibit greatest absorption at heights where the gas has very little vertical velocity but less where it has large blueshifting velocities, resulting in $\vee$ -shaped bisectors. Hence, the combination of these properties generally results in a $\subset$ rather than a $\supset$ shape for bisectors of moderately strong lines, as the weaker shape dominates near the continuum whereas the stronger shape dominates in the deepest areas. These relationships between bisector shape, strength and formation depth are alluded to by Asplund et al. (2000b). Obviously this entire situation would be reversed were the intergranular lanes to dominate the solar surface. Therefore, in the case of some strong lines where absorption in the *lanes* also contributes to the bisector shape, given that the contribution occurs high in the atmosphere, a redshifted $\wedge$ -shape will also play a significant role in the averaging. This adds to the contribution of the same $\wedge$ -shape by gas low in the granules and enhances the ‘turning-back’ of the top of the $\subset$ shape. These effects are crucial in understanding the results of Chapter 7.

3.3.2 Energetic Structure

The continued circulation of the fluid is driven by the rapid cooling via emission of radiation by the upflowing gas as it turns and diverges. The resulting gas entering the intergranular lanes is cool, dense and low in entropy. This causes it to drop quickly back towards lower heights, thereby forcing warmer gas up by mass conservation to continue the process.

The resulting borders between granules and lanes exhibit large gradients in entropy, density and temperature, producing a sharp intensity contrast between the two areas, as seen in Fig. 3.1 especially before instrumental correction. Fig. 3.4 illustrates the steepness of these temperature and intensity gradients. Note that the intensity does not quite track the temperature despite the assumption of LTE. In the granule centres, this is because energy transport is inhibited by the reduced velocity of upflowing gas (as discussed in the previous section). At the edges of granules, the same thing occurs due to the interaction of the strong upflowing and downflowing velocity fields, causing some vorticity in the boundary area and thereby inhibiting energy transport.

Figure 3.4: Temperature and emergent intensity along a slice of simulation at the solar surface ($\langle\tau\rangle = 1$), showing the steepness of the gradient between granules and lanes. Notice that intensity is reduced over the large granule centre, and does not increase quite so sharply at granule edges as temperature. (Figure taken from Stein & Nordlund 1998)



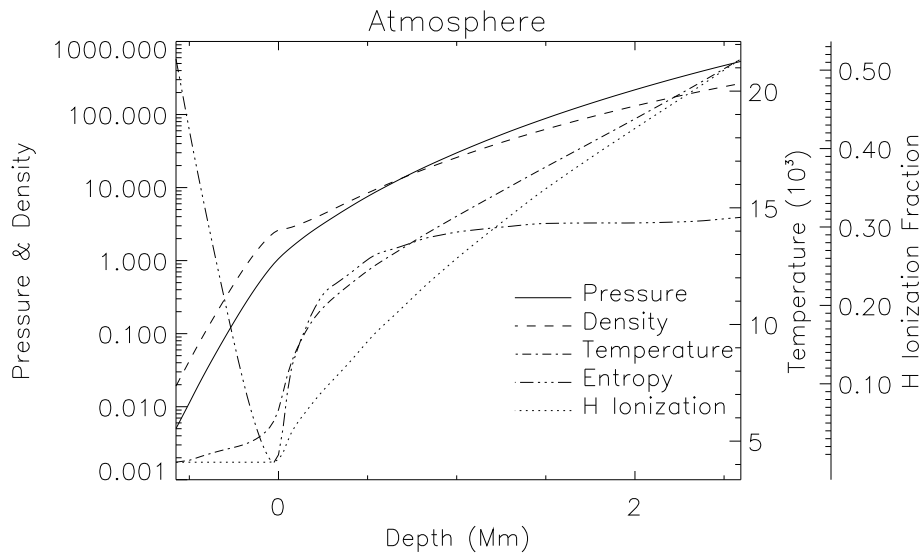


Figure 3.5: Mean features of atmosphere and upper convection zone produced by 3D convective simulations. (Figure taken from Stein & Nordlund 1998)

3.3.3 Mean Features

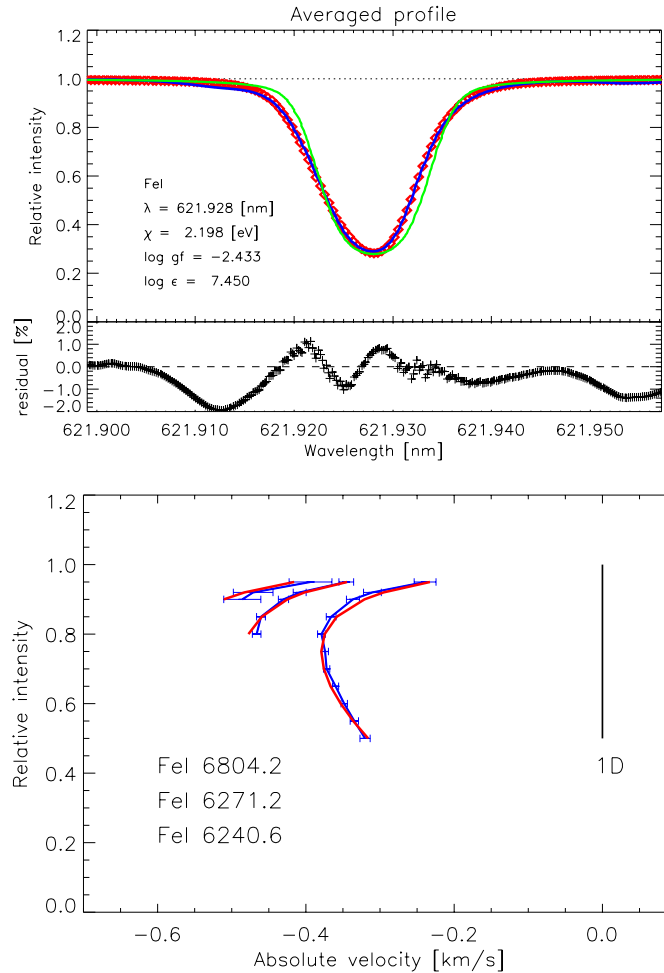
The run of assorted atmospheric properties with geometric depth is shown in Fig. 3.5, averaged over time and each horizontal plane. Density and pressure show a steady decrease across all heights, whilst temperature and hence entropy drop drastically across the surface of unit optical depth as the gas becomes clear and energy is released via radiation. In the photosphere temperatures remain comparatively constant, resulting in increasing entropy with height above the surface due to the steady decrease of pressure and density. In the subsurface regions entropy is close to constant, as temperature varies approximately with density and pressure. Hydrogen ionization steadily decreases outwards with the dropping temperature, to the point of essentially full recombination where the gas becomes optically thin.

3.4 Specific Results

3.4.1 Iron

One of the showpiece applications of the new convective models has been to solar Fe I and Fe II absorption lines (Asplund et al. 2000b,c). Both strong and weak lines were computed using the method described in §3.1 and §3.2, and the line profiles and bisectors compared to solar observations. As can be seen clearly in the examples of Fig. 3.6, the agreement was remarkably good. One of two highly significant results of these studies was to show that the 3D models did in fact correctly describe the convective process to the point of deriving the previously heuristically-achieved microturbulence and damping parameters. That is, the effects produced by the introduction of these free parameters in 1D were achieved naturally in 3D, without their inclusion at all. The other very significant result of the studies was to revise the solar iron abundance, something dealt with in §5.2. The convective models have also been applied with great success (Allende Prieto et al. 2002a) to the reproduction of Fe lines in the observed spectrum of the star Procyon.

Figure 3.6: Representative spatially and temporally averaged Fe line profile (upper) and bisectors (lower) calculated using 3D hydrodynamical model atmosphere (red, convolved with a sinc function to simulate instrumental effects cf. Chapter 6) compared to observation (blue). The modelled profiles and bisectors fit the observations almost perfectly; residual intensity is shown in the upper frame to illustrate the small remaining discrepancy. Also shown are the 1D bisector and best fit HM line profile (green, $\xi_t = 0.845 \text{ km s}^{-1}$, $V_{mac} = 1.6 \text{ km s}^{-1}$, $\log \epsilon_{\text{FeI}} = 7.60$), clearly producing an inferior fit to the observations. (Figure taken from Asplund et al. 2000b)



3.4.2 Silicon

In parallel with the aforementioned solar Fe studies, solar Si lines were calculated and compared to observation. Again, the agreement was excellent (Fig. 3.7). Also again, the three-dimensional models produced a shift in the derived elemental abundance (see §5.2). The significance of this though was not so much in the replication of Si lines and associated abundance determination *per se*, but in the fact that Si is used as a common reference element between the Sun and meteorites. Hence, the revision in the solar Si abundance corresponded to a similar shift in all previously derived meteoric abundances, bringing near perfect agreement between the newly derived solar Fe abundance and the revised meteoric Fe abundance. This shift in meteoric abundance scale should have quite broad implications for theories of solar system and planetary formation, as will also be true of the current study and discussed in §5.3 and §8.6.

3.4.3 Oxygen

More recently, the models have been applied to forbidden and allowed oxygen ([O I] and O I) and OH lines (Allende Prieto et al. 2001; Asplund et al. 2004c). This time however, accurate reproduction of the O I line profiles required the use of NLTE calculations (Fig. 3.8). LTE hydrodynamical and radiative transfer simulations were carried out over the entire simulation timeframe, followed by NLTE radiative transfer over two (highly temporally

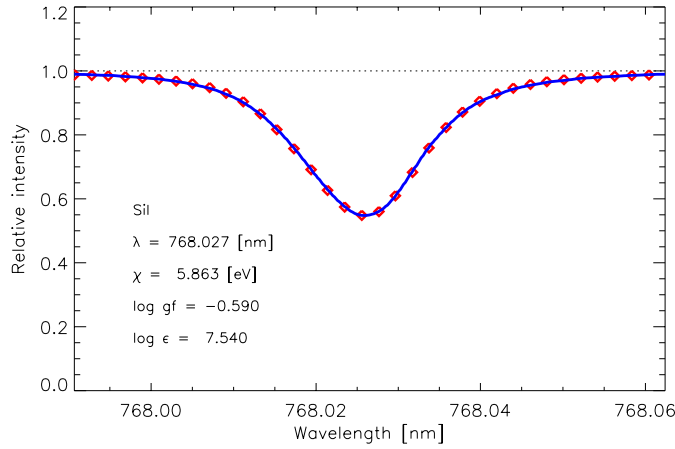


Figure 3.7: Representative spatially and temporally averaged Si line profile calculated using 3D model atmosphere (red) compared to observed profile (blue). Again, the agreement is excellent. (Figure taken from Asplund 2000)

separated) snapshots for each O I line. The difference for each individual line between the LTE and NLTE profiles in the particular snapshots chosen was then added to the fully averaged profiles to produce the 3D NLTE line profile. In this way, a new solar oxygen abundance was calculated (cf. §5.2) using the NLTE O I and LTE [O I] and OH lines. The new oxygen abundance resolved a long-running discrepancy between solar and local ISM determinations. This new value is particularly significant for the study of Chapter 8 in that it allows oxygen abundance to be accurately fixed and carbon abundance varied in the analysis of CO lines.

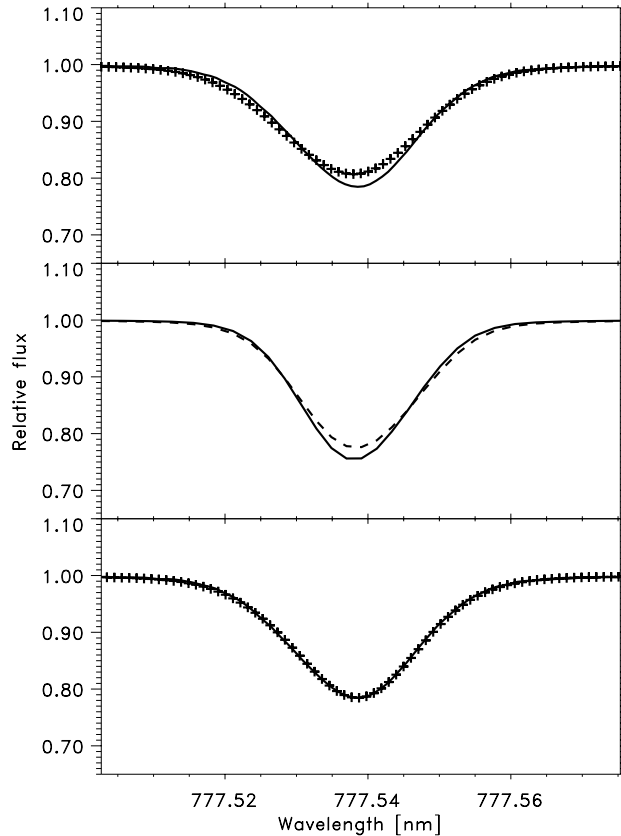


Figure 3.8: *Top:* Spatially and temporally averaged 777.53nm O I line calculated using 3D LTE model atmosphere (+) compared to observed profile (solid). *Middle:* The same line, spatially averaged and calculated over a single snapshot in NLTE using the 3D atmosphere (solid) compared to the 3D LTE profile of the top panel (dashed). *Bottom:* Fully averaged 3D LTE profile of top panel multiplied by the ratio of the LTE and NLTE profiles in middle panel (+) compared to observation (solid). Clearly NLTE effects are important, with excellent agreement between the final model output and the observed spectrum. (Figure taken from Asplund et al. 2004c)

3.4.4 Beryllium and the Missing UV Opacity

The solar UV flux has always been lower than that predicted by various atmospheric models (e.g. Vernazza et al. 1976). As yet unquantified metal absorption lines were in the past typically invoked as explanation of this fact, though calculations using modern lists of UV metal absorption features fail to reproduce the observed spectrum (Allende Prieto et al. 2003). In order to quantify the missing opacity, the oxygen abundance derivation explained in the previous section was used (Asplund 2004) to fix the abundances indicated by OH lines in the UV section of the solar spectrum. Compensating for this missing opacity, a Be II line was used to determine the solar beryllium abundance (cf. §5.2), which was in agreement with the meteoric Be abundance. This result confirmed the findings of a previous 1D study (Balachandran & Bell 1998), showing unequivocally that there was indeed approximately 50% more opacity present near 310 nm than predicted by metallic absorption lines alone. This demonstrated that the missing opacity can likely be identified with photoionization of Fe I, as suggested by calculations by the Iron Project (Hummer et al. 1993; Bell et al. 2001). The demonstration of agreement between photospheric and meteoric Be abundances also has implications for theories of stellar element processing, as though it is known that lithium has been depleted over the Sun's lifetime, it appears that other light elements such as Be and B have not (Asplund 2004).

3.4.5 Comparisons with Helioseismology

Helioseismology is concerned with the analysis of solar oscillations, providing information about the Sun's internal structure. For the most part, the findings have agreed remarkably well with the predictions of the Standard Model (di Mauro 2003). In the outer third of the Sun's radius, where the Standard Model is lacking, comparisons are apt between the 3D convective models and the findings of helioseismology. Such comparisons have been performed by Rosenthal et al. (1999) with regard to the frequencies of the eigenmodes of the p mode (pressure driven, as opposed to gravity driven) solar oscillations. They found that the traditional mixing length theory overpredicts the observed frequencies, but that the agreement of 3D hydrodynamical models with observations is far better. This is due to an upwards shift of constant pressure surfaces (responsible for acoustic wave reflection) in the 3D models relative to their locations in mixing length models, extending the resonant wavelengths of the p modes. Trampedach et al. (2003) showed that these results could be used to derive the depth of the solar convection zone: $28.61 \pm 0.02\%$, in excellent agreement with helioseismic observations. These findings lend credence to both relatively young fields.

However, as noted in both papers (Rosenthal et al. 1999; Trampedach et al. 2003), there is still some disagreement between the modelled and observed frequencies. An improved formalism for comparison of the 3D models with helioseismology was developed by Nordlund & Stein (2001), and it is anticipated that this will assist in resolving the discrepancy in the near future. A recent paper identifying areas for improvement in helioseismology (Boothroyd & Sackmann 2003) cited uncertainties in traditional C, N and O photospheric abundances as currently the largest sources of error in helioseismological analyses. One might expect that recent re-evaluation of these abundances (§3.4.3 & §3.4.7) will do much in this respect, furthering the contribution of the Stein-Nordlund models to this field.

However, a major discrepancy actually exists between the observations of helioseismology and the new solar metallicity implied by the assorted revised elemental abundances

(Asplund et al. 2004c). This is because the new solar metallicity ruins the previous agreement between the helioseismically-derived and the Standard Model-derived interior sound speeds. This metallicity difference also implies that solar and protosolar cloud helium abundances must change from the currently accepted values. It is not exactly clear where the resolution to this problem lies, but efforts are currently directed toward finding out.

3.4.6 Limb Darkening

The limb-darkening effect occurs due to the optically thin upper layers of the atmosphere. A line of sight originating from the edge of the solar disc will ‘graze’ the upper layers of the atmosphere without passing any lower, such that optical depth unity in the direction in question will occur at some point rather high up in the atmosphere (though through a large geometrical length of gas). Temperatures being lower at such heights, the continuum observed will be less bright, and the solar ‘limb’ is seen to be reduced in brightness relative to the rest of the solar disc. This effect was investigated (Asplund et al. 1999) using the 3D models, with the temperature inhomogeneities made possible in 3D seen to allow limb darkening to occur far more realistically than in 1D models (Fig. 3.9). Using the same NLTE technique discussed in §3.4.3, centre to limb variation of O I lines was investigated (Allende Prieto et al. 2004) and found to agree with observed limb darkening.

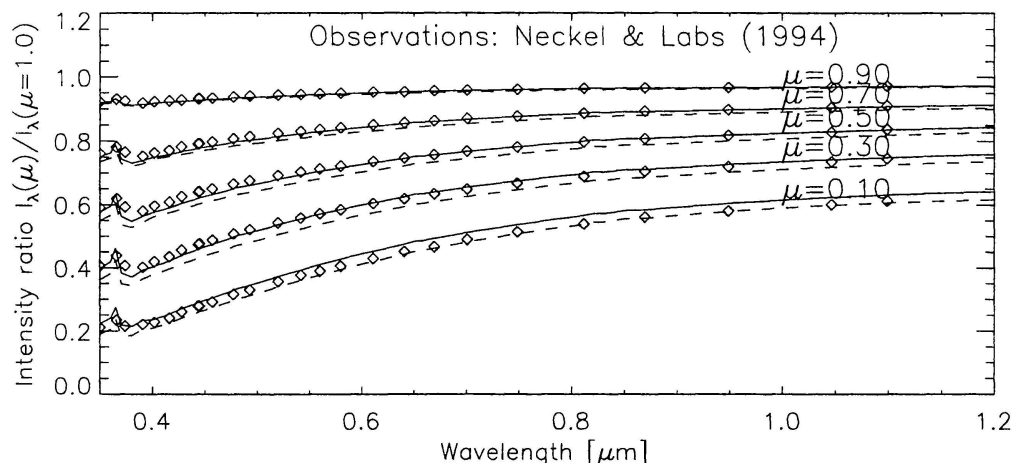


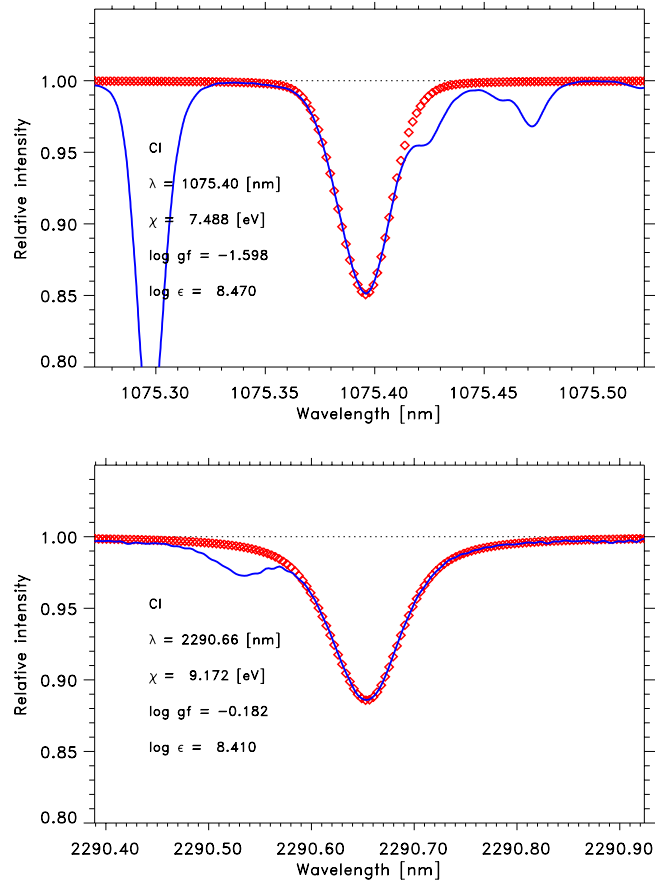
Figure 3.9: The observed limb-darkening curves (diamonds) in comparison with the predictions of Stein-Nordlund (solid) and MARCS (dashed) models. The centre to limb behaviour is well reproduced by the 3D model, in contrast to the overprediction of the limb-darkening effect by the 1D model. (Figure taken from Asplund et al. 1999)

3.4.7 Carbon & Nitrogen

Almost in parallel with the current study have been analyses of [C I] (Allende Prieto et al. 2002b; Asplund et al. 2004a), C I, CH, C₂ (Asplund et al. 2004a) and CN lines (Asplund et al. 2004b), bringing further ratification of the 3D models (Fig. 3.10) and revised carbon and nitrogen solar abundances (cf. §5.2). C I line abundances were corrected for NLTE effects, though this time using an abundance correction based upon 1D NLTE calculations rather than a profile change from representative 3D calculations, owing to the number of energy levels required in a NLTE calculation of carbon. The findings

with respect to carbon in particular have important ramifications for the interpretation of results from the current study; specifically, they provide a comparison for the solar carbon abundance determination to be carried out using CO lines.

Figure 3.10: Representative spatially and temporally averaged C I line profiles calculated using 3D LTE model (red) compared with observed spectrum (blue). The agreement is again very good. Correction factors of ≈ 0.05 dex were derived from 1D NLTE calculations and applied to the abundance indications of all lines such as these. (Figure taken from Asplund et al. 2004a)



The COndrum

The investigation of carbon monoxide absorption lines to date has been like a thirty-year attempt by a dozen people to simultaneously unravel an enormously knotted ball of yarn, each speaking a different language. This chapter will outline why CO has caused such confusion, the great debates that it has sparked and the projected way forward. It should be made clear at this point that the features referred to in virtually every paper on the topic are those arising from vibration-rotation transitions, characterised by changes in rotational (J) and vibrational (ν) quantum numbers. The selection rules for such transitions are $\Delta J = \pm 1$, $\Delta \nu = 0, \pm 1, \pm 2, \pm 3 \dots$ (Dopita & Sutherland 2003); the lines discussed are typically those with $\Delta \nu = 1$. Lines having $\Delta J = 1$ are referred to as part of the **R branch**, and those of $\Delta J = -1$ are of the **P branch**. Transitions are identified in the form

$$\nu_{final} - \nu_{initial} \ B J_{initial},$$

where B is the branch, such that ‘7-6 R68’ would refer to a transition from $\nu = 6, J = 68$ to $\nu = 7, J = 69$. As a molecule, CO concentration is subject to the highly temperature dependent balance between formation and dissociation. The high dissociation energy of the CO molecule makes it a good probe of low temperature areas in stars, as the balance between CO formation and destruction undergoes its most marked shift at temperatures too high for most other molecules to exist. This means that of all molecules present in the Sun’s atmosphere, CO is the most sensitive to temperature variation. Finally, vibration-rotation CO lines exist exclusively in the infrared section of the spectrum.

4.1 Early Observations of CO in the Sun

The first observations of CO lines in the Sun were performed by Noyes & Hall (1972). These observations represented something of a bombshell: measurements of $\Delta \nu = 1$ lines taken near to the solar limb exhibited core brightness temperatures¹ ($\approx 3700\text{K}$) *below* the classical temperature minimum of 4500K thought to exist at the top of the photosphere. Noyes & Hall attributed this anomalous behaviour to cool lanes evident in the solar granulation pattern, not realising that their observations were likely probing areas somewhat above the classical temperature minimum.

¹The brightness temperature of a line is defined as the temperature of a black body required to produce the observed line intensity (Dopita & Sutherland 2003). The corresponding height of line formation is arrived at by the adjustment of the temperature structure in a model to best reproduce the observed line core depths (e.g. Ayres & Testerman 1981; Noyes & Hall 1972), and is hence highly model dependent. This should be kept in mind throughout the ensuing discussion.

The roots of the entire CO controversy can be traced back to a debate that was occurring around this time as to the true photospheric temperature minimum, between Thomas Ayres and collaborators and Jorge Vernazza, Eugen Avrett and their collaborators at Harvard. At the time, debate centred on whether the temperature minimum at the top of the photosphere was 4400-4500K, on the basis of the damping wings of Ca II and Mg II lines (Ayres & Linsky 1976), or 4200K on the basis of the ultraviolet continuum (Vernazza et al. 1973). Strangely enough, the results of Noyes & Hall were largely ignored by the community at the time, treated as “... a minor oddity of the atmosphere ...” that would hopefully eventually just go away (Ayres & Rabin 1996).

Almost a decade later, with debate ongoing as to the actual temperature minimum, the attention of Ayres & Testerman (1981) was drawn to CO as a temperature probe. They examined $\Delta\nu = 1$ and $\Delta\nu = 2$ bands using a newly developed Fourier transform spectrograph (**FTS**, explained in Chapter 6). Expecting the CO temperature indications of Noyes & Hall (1972) to fall into line with other diagnostics under the weight of their improved instrumentation and analysis, Ayres & Testerman were rudely surprised when their off-disc measurements unequivocally confirmed those of Noyes & Hall. In fact, their findings were most naturally explained by the absence of a photospheric temperature minimum, requiring an outwardly decreasing temperature structure from the base of the photosphere right through the chromosphere; i.e. no chromosphere at all!

However, given that unlike their absorption wings, the Ca II and Mg II line cores showed *emission* indicating chromospheric temperatures well above the classical minimum (Ayres & Linsky 1976), some kind of chromosphere had to exist. The CO absorption lines however, required the rather drastic step of discarding the chromospheric temperature rise at greater heights, in conflict with the Ca II/Mg II emissive cores. Clearly something was wrong, and even at this early stage Ayres & Testerman (1981) recognised the need for multidimensional models, commenting that single-dimensional models “... may have limited applicability,” in the case of the solar atmosphere.

As a solution, they put forward the idea that the area around the photosphere-chromosphere transition was “thermally bifurcated”. Ayres (1981) proposed the existence of some sort of cool CO structure in the low chromosphere, coexistent with other areas of hotter gas responsible for the Ca II and Mg II core emission. The mechanism proposed for the lower fork of this bifurcation was radiative cooling by CO itself via the $\Delta\nu = 1$ lines, causing temperatures to drop below 4000K locally. Ayres showed that this was an equilibrium stable against relatively large mechanical perturbations. He went on to show that if enough mechanical energy were deposited in the gas to raise the temperature sufficiently to denature most of the highly temperature-sensitive CO, H^- ions would act as heating rather than cooling agents until the gas reached a critical temperature of 4900K, at which point they would have the opposite effect. The mechanism proposed for this upper fork was the deposition of mechanical energy in small areas of the chromosphere by magnetic flux tubes, already possibly associated with the hot Ca II and Mg II emission lines (Skumanich et al. 1975).

The introduction of this inhomogeneity also solved the problem of the different temperatures derived from the damping wings and the UV continuum, though later revisions of the VAL (Vernazza-Avrett-Loeser) 1D semiempirical model (Vernazza et al. 1976, 1981) did allow for some rise in its predicted temperature minimum. The VAL model has always had problems though, despite being based on some very elegant NLTE results. It can’t describe solar properties accurately across the wavelength range (Harris et al. 1987),

abundances derived using it² show greater wavelength dependencies than other 1D models (Grevesse et al. 1984; Goldman et al. 1983; Harris et al. 1987) and the entire concept of using the UV continuum to calibrate its temperature structure is flawed owing to the missing UV opacity described in §3.4.4³. The focus on the VAL model is not merely incidental; despite its shortcomings, much of the early (and even some of the very late) debate about CO lines was performed with reference to VAL.

The next piece in the puzzle was provided by Ayres & Wiedemann (1989), who tested the assumption of LTE used in the thermal bifurcation model. It was found that departures from LTE had less than a 2% effect upon CO line cores, even as near to the solar limb as $\mu = 0.1$. This was a very important result, as NLTE scattering events could not be invoked to suggest that CO line depths were under-representing the local temperature in the low chromosphere, whatever the model considered. Such a finding bodes well for the LTE calculations intended in the current study.

Hot on the heels of the NLTE results firming the bifurcation model came a more detailed calculation of CO cooling rates (Mauas et al. 1990). By taking into account the effect of the increase in optical depth caused by raised local concentrations of CO, the authors suggested that the CO cooling advocated by Ayres (1981) was not likely to produce quite such cool, stable clouds as predicted. Whilst the VAL model was the backdrop for these results, the calculations were also carried out with a version containing modified temperature minima and ‘absent’ chromospheres (à la Ayres 1981), producing qualitatively the same result. The existence of some cool CO in the atmosphere was not disputed however, and the temperature inhomogeneities were suggested as possibly due to the effects of localised mechanical heating alone. However, the suggestion by Mauas et al. of such “... reduced chromospheric heating in some regions...” in fact contradicts the fundamental concept of the chromosphere according to VAL: that is, the chromospheric temperature rise is ubiquitous. If it were the case that the chromospheric heating mechanism operated over the entirety of the chromosphere, without inhomogeneity, CO cooling would be necessary to cause bifurcation. However, if it were that chromospheric heating was in fact a *local* phenomenon as suggested by Mauas et al. to explain the cool CO cores, then CO cooling would not be needed for bifurcation to occur and the VAL model’s chromospheric temperature structure would indeed be *wrong*. In attempting to debunk the bifurcation theory by disproving the CO-cooling proposition, the authors in fact ended up bolstering the bifurcation *concept* by suggesting a more natural dynamical mechanism for it, in the process discrediting their own model’s chromospheric temperature structure.

The presence of cool CO in the chromosphere was put beyond a doubt four years later with the startling discovery of *emission* in the $\Delta\nu = 1$ line cores in the very low density region beyond the solar limb (Solanki, Livingston, & Ayres 1994). Thanks to an upgraded spectroscope, these observations were able to probe even higher layers than Noyes & Hall (1972) or Ayres & Testerman (1981) had ever been able to, finding significant amounts of CO as high as 900 km above the surface. As with other CO diagnostics, the emission cores exhibited a brightness temperature of less than 4000K despite the surrounding chromospheric gas of over 6000K. These findings indicated that the low chromosphere did in fact exist in two thermal states: a warm one responsible for traditional temperature measure-

²As mentioned earlier, how this is done is explained in §5.1

³The VAL model atmosphere was thought to have the effects of the missing UV opacity mostly accounted for by its inclusion of the metal lines suspected at the time to be responsible for the reduced UV continuum (Vernazza et al. 1976); the rest of the lines were not thought necessary. It therefore contained no opacity multiplier in the UV, and we now know from the arguments in §3.4.4 that this treatment is incorrect.

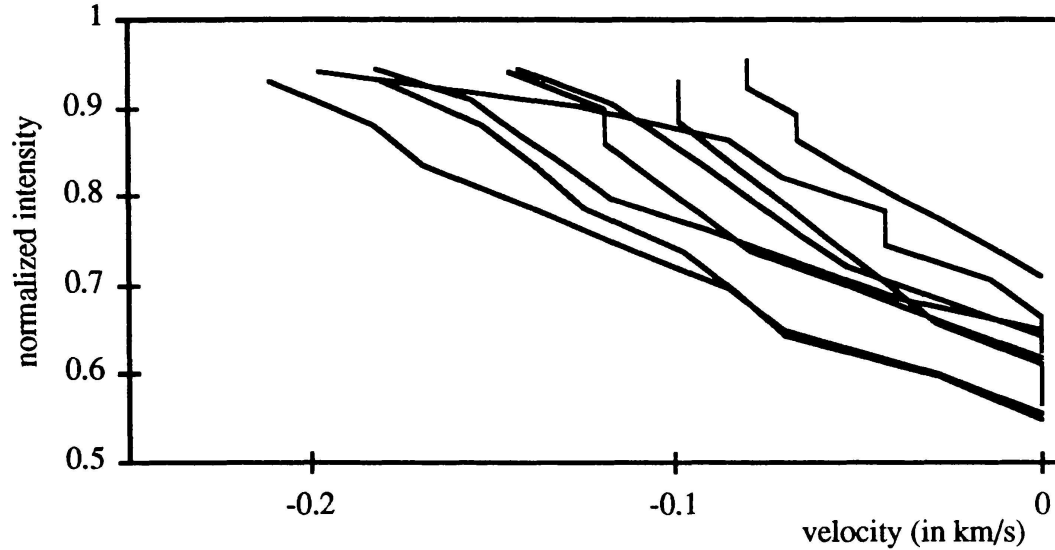
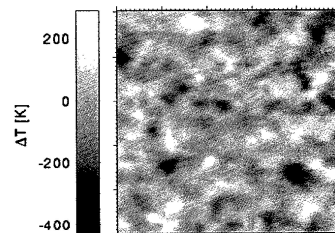


Figure 4.1: Strong solar CO absorption line bisectors extracted from an early ATMOS mission, showing granular formation signatures. Bisector feet have been artificially shifted to 0 km s^{-1} . (Figure taken from Blomme et al. 1994)

ments and a cool CO-bearing one whose temperature structure underwent a sharp jump to normal chromospheric values between 900 and 1100 km. This supported the notion of bifurcation, though said nothing about the physical mechanism behind it.

Separate to the entire temperature debate, Blomme et al. (1994) performed the first analysis of CO lines in the ATMOS solar spectrum (cf. Chapter 6), and the only measurement of solar CO line bisectors prior to the current study. Their work was very preliminary; more substantial work had been published on CO bisectors in *other* stars (Tsuji 1991), but some interesting results were produced nonetheless. The resulting strong line bisectors (Fig. 4.1) can be seen to show a definite bluewards ($\searrow$) tilt, indicating that the lines have been formed very high in upflowing granules. This is as one might expect, considering the contrast inversion reflecting the low temperatures over granules described in §3.3.1.

Figure 4.2: Temperature heterogeneity in the quiet Sun (away from explosive events, sunspots, etc.) as seen in the core of the 3-2 R14 CO line. Notice temperature fluctuations of up to 600K. (Figure taken from Uitenbroek et al. 1994)



Using imaging spectroscopy, Uitenbroek et al. (1994) studied spatial and temporal variations in CO absorption at disc centre, as well as confirming the stunning off-limb observations of Solanki, Livingston, & Ayres (1994). The temporal and spatial variation at disc centre displayed temperature inhomogeneities of up to 600K (Fig. 4.2) at the heights of formation of the stronger lines. The variation in temperature was found to be correlated with hydrodynamic perturbations, predominately of high frequency p mode but possibly also convective origin. ‘High frequency’ p modes refer to those of 3-5 minute period ‘trapped’ in the convective envelope, whilst other modes of wavelength longer than

the depth of the convection zone cannot become trapped. This result supported the existence of the temperature bifurcation, though driven by dynamic processes as per the suggestion of Mauas et al. (1990) rather than CO cooling and magnetic heating as per the original concept (Ayres 1981).

In light of findings over the previous 10 years, Ayres & Rabin (1996) revisited the idea of bifurcation. They re-derived the CO cooling function disagreed on (Ayres 1981; Mauas et al. 1990), getting around the problem raised by Mauas et al. of optical thickness due to CO formation by claiming that CO cooling is in fact most efficient at intermediate rather than low optical depths. Not surprisingly, they confirmed Ayres' original conclusion that CO cooling was the most important process in the apparent bifurcation occurring in the lower chromosphere. They also performed similar observations to Uitenbroek et al. (1994), reporting off-limb emission to heights of 850 km and spatially and temporally resolved disc centre images indicating some correlation between high frequency dynamic processes and CO absorption. The spatially resolved data showed isolated bright points correlated with emission in the cores of the Ca II and Mg II lines, uncorrelated with the observed high frequency p modes. Ayres & Rabin (1996) hence inferred the existence of a pervasive 'COmosphere' below 850 km, modulated slightly but relatively unaffected by the 3-5 minute oscillations and interspersed with small hot grains showing Ca II and Mg II emission.

Though not identified by the authors, this picture strongly concurred with earlier observations by Lites et al. (1993), whom had shown Ca II and Mg II emission to be spatially isolated rather than horizontally uniform. According to Ayres & Rabin, the entire pattern was due to the CO cooling originally advocated by Ayres (1981), punctuated in certain areas where sufficient energy had been input to disable the cooling mechanism. Magnetic flux tubes had by this time been all but discarded as the mechanism for this departure, and though the subject was not discussed, a parting statement by the authors flagged upcoming simulations by Carlsson & Stein as a possible way forward in this respect.

4.2 The Debate Heats Up ...

The mid-to-late nineties saw some new players take the field in the grudge match between the Ayres and Harvard camps, with Mats Carlsson and Bob Stein weighing in on the Ayres side, Wolfgang Kalkofen and Peter Ulmschneider on the Harvard team and Han Uitenbroek⁴ playing a relatively neutral role.

Carlsson & Stein (1995, 1997) provided probably the most controversial input to the whole debate yet with their demonstration that the Ca II 'H_{2ν}' and 'K_{2ν}'⁵ grains are formed by acoustic shocks. They simulated H_{2ν} and K_{2ν} grain formation using a one-dimensional ab initio model based upon the NLTE solution to the 1D version of Eq. 3.1-3.3. They drove low frequency p mode acoustic waves through the models from the bottom of the simulation domain using an artificial piston whose driving frequency was coupled to the observed period of oscillation of an Fe I line, formed at a height of approximately 800 km. Upon reaching the middle chromosphere (800-1000 km), the acoustic waves formed shocks in the low density gas, heating and compressing regions enough to facilitate the lighting up of the grains. Carlsson & Stein found that whilst they are not directly responsible for

⁴incidentally, also at Harvard

⁵'H' and 'K' are just different Fraunhofer designations, whilst '2ν' refers to the location of the emission line in the broad H or K Ca II absorption profile

the bright grains, the interaction of the high frequency trapped p modes with the lower frequency acoustic waves is what causes their localised nature and governs their horizontal distribution. These findings strongly supported the notions of a bifurcated atmosphere with differences caused by dynamic effects pushed by Ayres & Rabin (1996), even also suggesting some influence by CO cooling owing to the inclusion of ICE CO opacity in the model via the Uppsala opacities and equation of state. The major implication of this work was that on average, there is no chromospheric temperature rise at the top of the photosphere.

Possibly at odds with the findings of the H and K grain simulations were observations by Carlsson, Judge, & Wilhelm (1997) using the SUMER instrument aboard the SOHO satellite. They observed chromospheric lines in emission “... everywhere, all of the time,”, apparently contradicting the picture produced by the piston model of a cool lower chromosphere interspersed with hot grains. However, the SUMER instrument probed the chromosphere above 1000 km, so was not sensitive to the proposed low temperature region (Ayres 2002), picking up more grains than the model had predicted for the region below 1000 km. It was noted (Carlsson, Judge, & Wilhelm 1997) that the model would need improvements, such as the introduction of magnetic fields, to be able to reproduce these features of the upper chromosphere where the traditional dual mechanism of dynamical and magnetic heating reigns.

Kalkofen, Ulmschneider, & Avrett (1999) however picked up upon the perceived discrepancy between the models (Carlsson & Stein 1997) and observations (Carlsson, Judge, & Wilhelm 1997), launching a scathing attack upon the conclusions of Carlsson & Stein (1995, 1997). Their fundamental argument against the Carlsson-Stein model was that it did not adequately represent the entire solar energy output, neglecting energy input to the chromosphere by assorted high frequency acoustic waves and therefore failing to reproduce the observations of ubiquitous chromospheric emission. The absence of magnetic fields in the Carlsson-Stein model and the fact it had not been designed to reproduce such observations was not identified. The discussion of the assertions of this paper will be left to those below regarding a followup paper (Kalkofen 2001) and a later rebuttal by Ayres (2002).

An aside to the raging argument was the presentation of Hamilton & Lester (1999). They studied the line depth, wavelength and excitation potential dependence of observed shifts in a large sample of CO lines. Their results confirmed those of Blomme et al. (1994), essentially just showing that CO absorption occurs predominantly in upflowing granules, with different velocities observed for lines of different formation depth.

The next phase in the CO argument was brought by Uitenbroek, performing detailed 1D NLTE (Uitenbroek 2000b) and relatively low-detail 3D LTE (Uitenbroek 1999, 2000a) simulations of CO absorption in the solar disc. Using a single snapshot from an early version (Stein & Nordlund 1989) of the Stein-Nordlund models, Uitenbroek (2000a) calculated a spatially averaged spectrum and granulation pattern for a series of $^{12}\text{C}^{16}\text{O}$ and $^{13}\text{C}^{16}\text{O}$ lines. The granulation patterns in the line cores showed an inverted intensity contrast, demonstrating the increased absorption and presence of CO in the cool zones above the granular centres, seen in the modelled CO distribution of Fig. 4.3. Observations of the granulation pattern in the line cores demonstrated the same, though were of lower contrast even after the model output had been corrected for instrumental and seeing effects. Correspondingly, the calculated line profiles were deeper than those seen in the ATMOS solar spectrum (refer to Chapter 6). This lead Uitenbroek (2000a) to the conclusion that the 3D simulations exhibited too much CO due to the assumption of ICE (Instantaneous

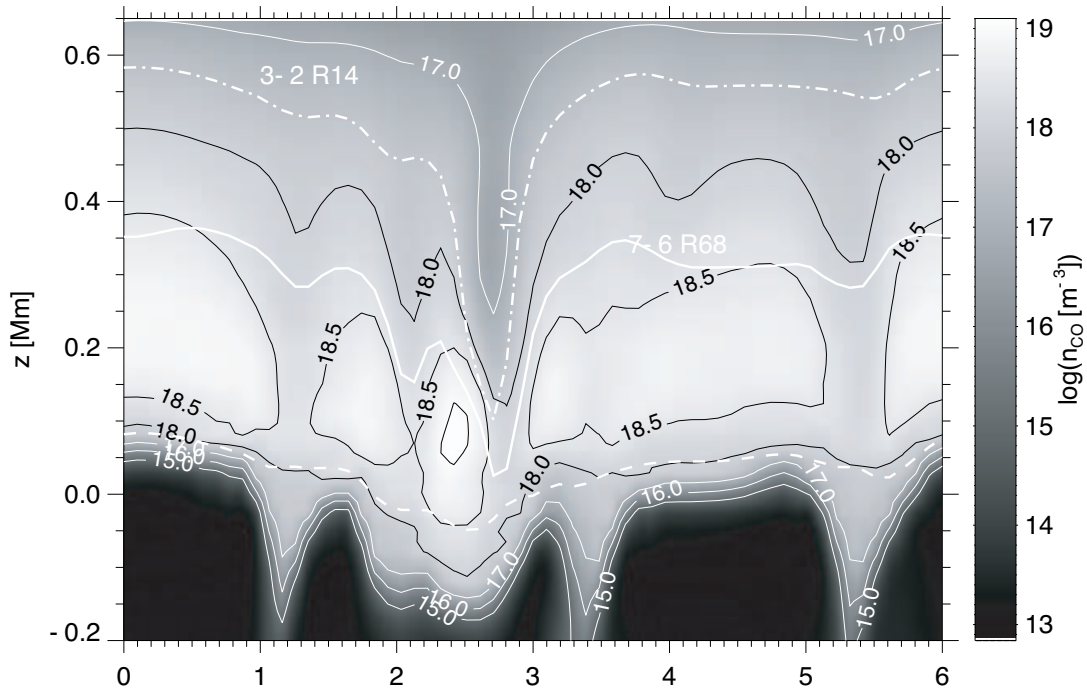


Figure 4.3: CO concentration shading and contours across a vertical slice through an early 3D simulation of CO line formation in the solar photosphere. The dashed, solid and dot-dashed white lines indicate optical depth unity for the IR continuum, 7-6 R68 and 3-2R14 CO lines respectively. Note the enhanced CO density over granule centres. (Uitenbroek 2000a)

Chemical Equilibrium); if ICE was not assumed, CO would not form so quickly above the granules and the results would be better matched to observation.

Despite the failure of a preliminary version of the 3D models to describe disc-centre CO line formation, this was at least a promising result, as every otherwise self-consistent model atmosphere to this point⁶ had always under-predicted CO absorption due to their chromospheric temperature rises. The 1D NLTE results of Uitenbroek (2000b) supplemented this work, reconfirming more accurately Ayres & Wiedemann’s (1989) finding that the CO line cores were formed fully in LTE. Uitenbroek (2000b) here also drew similar conclusions as to the ICE assumption, this time based upon overestimations of CO line core temporal variations compared to observation. The author also concluded that the use of 3D rather than 1D modelling is imperative in future analyses, owing to the horizontal inhomogeneity inherent in the solar atmosphere.

Kalkofen (2001) continued his attack upon the Carlsson-Stein models, deriving quantitative discrepancies between the output of models and observations based upon his prior qualitative objections. A proper discussion of the inconsistencies, misrepresentations and fallacies presented in this paper would itself be a full-length document, but a very brief discussion of some points not discussed below as explicitly dealt with by Ayres (2002) will be entered into. Kalkofen (2001) argues against the cool chromospheric structure in the Carlsson-Stein model at one stage simply on the basis that it “... is fundamentally different from the temperature structure of the earlier models,” and “... would not resemble the VAL models.” This is the exact point of contention, and it is a clear truism to imply

⁶i.e. not including those based purely on CO and neglecting other lines like the models of Ayres (1981); Ayres & Testerman (1981); Solanki, Livingston, & Ayres (1994) and (Ayres & Rabin 1996).

that to disagree with his viewpoint is by definition incorrect. He also attempts to make the point that the shocks formed in the Carlsson-Stein simulations would destroy all CO in the chromosphere given the high post-shock temperatures they cause, neglecting that in reality, owing to the spatial interaction with the trapped p modes such shocks are highly localised events, causing localised grain formation rather than shocking and heating the entire chromosphere. Obviously such spatial structure could not be expressed in a 1D model; the point of the Carlsson-Stein models was to show the mechanism for individual grain formation, not to suggest a horizontally homogeneous solution. Kalkofen (2001) also attempts to discredit the Carlsson-Stein view of a spatially differentiated lower chromosphere by citing figures from Carlsson, Judge, & Wilhelm (1997) that show 50% horizontal coverage by bright grains and corresponding figures from Solanki, Livingston, & Ayres (1994) showing up to 85% cool CO coverage, concluding that the grains and the CO lines must form at different heights and the lines must therefore form in the photosphere. The problem with this is that the Carlsson, Judge, & Wilhelm measurements probed areas above the Solanki, Livingston, & Ayres observations anyway, so there is no reason whatsoever that the lower grain filling factor derived by Carlsson & Stein (1997) in their simulations at the top of the proposed COmosphere cannot horizontally coexist with the large CO filling factor, whilst at greater height in the chromosphere proper, magnetic heating enhances the grain filling factor to that of Carlsson, Judge, & Wilhelm (1997).

Kalkofen et al.'s particular adherence to the VAL models as the semiempirical model of choice, over e.g. the HM model, is questionable at best given its inadequacies previously discussed in §4.1. Specifically, Kalkofen (2001) argues that given some very special conditions and additions, VAL *might* be consistent with the on disc measurements, but freely admits that “... the problem of the low-brightness temperatures seen at the limb remains.” He and collaborators conclude (Kalkofen et al. 1999) that the correct model is therefore “... incompatible with models in which the CO lines form at chromospheric heights,” seemingly implying that the limb and off-limb observations of Noyes & Hall (1972); Ayres & Testerman (1981); Solanki, Livingston, & Ayres (1994); Uitenbroek, Noyes, & Rabin (1994) and (Ayres & Rabin 1996) were all simply *wrong* because they did not agree with his preferred model.

Ayres took issue with much of Kalkofen et al.'s argument, commenting as to their failure to explain the observations of cool CO in the low chromosphere (Ayres 2000) before launching a full-scale attack on the fundamental principles upon which the Kalkofen papers were based. Ayres (2002) highlighted the mistaken identification by Kalkofen of the Carlsson-Stein model as semiempirical and therefore on a physically similar footing to the VAL model, spelling out the fundamental differences between the two approaches and the reasons this made the Carlsson-Stein model an inherently better test of the underlying processes it was designed for. He also went on to explain that the Carlsson-Stein model was only ever intended to simulate the formation of H and K grains, not reproduce the entire chromospheric spectrum as Kalkofen et al. demanded of it. Ayres reiterated the point of Carlsson, Judge, & Wilhelm (1997) that the model did not include magnetic fields so could not possibly hope to describe the chromosphere above 1000 km. As a result, he concluded that the observation by the same group of all chromospheric lines being always in emission is not at all contradictory to the COmosphere concept, as those observations probed hotter, traditional chromospheric regions above the proposed COmosphere. The modern structured paradigm alluded to in §2.2.1 and championed by Ayres and collaborators is shown in Fig. 4.4 alongside the traditional layered alternative preferred by the Harvard camp.

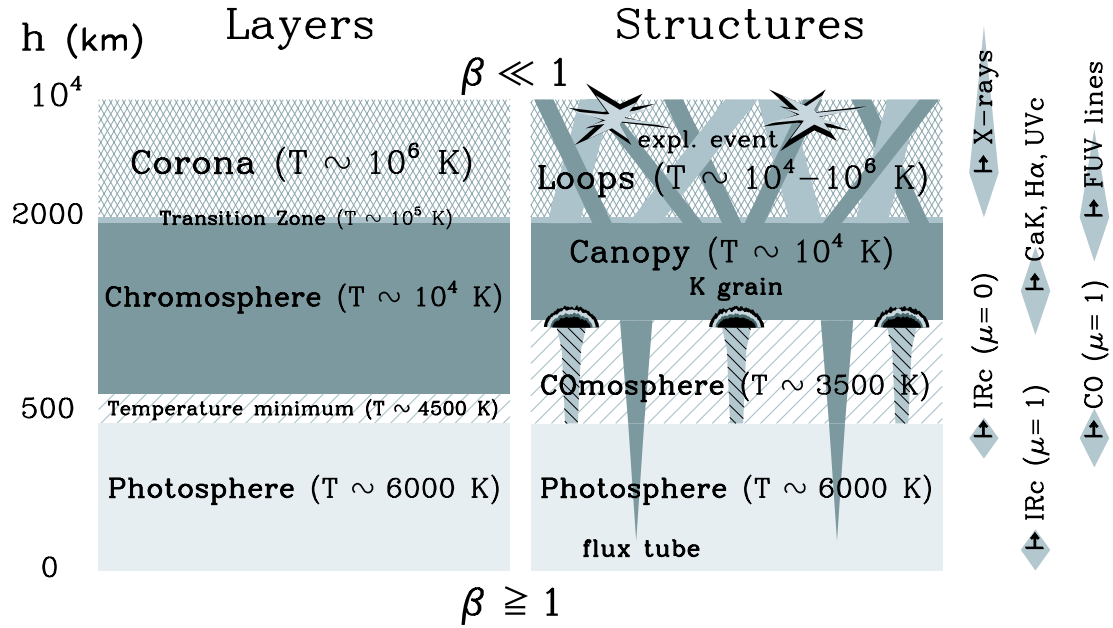
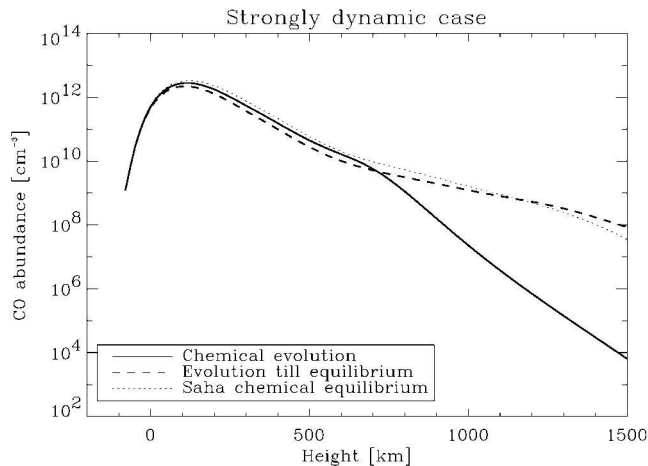


Figure 4.4: Conflicting views of the solar atmosphere: The traditional layered paradigm supported by Avrett, Kalkofen and others (left) and the modern, structured paradigm of Ayres and collaborators. β refers to the ratio of gas to magnetic pressure, and the formation heights of various spectral features are indicated on the right (where “c” means continuum). Not illustrated in the diagram is that the traditional picture is static whereas the structured model is implicitly time-dependent. (Figure taken from Ayres 2002)

Ayres (2002) tested the Carlsson-Stein model against freshly observed CO absorption and emission, where it was found to perform admirably given that it was never designed for this use, far outperforming the Harvard group’s VAL-derived model of choice. The Carlsson-Stein models were actually found to be not quite cool enough to properly describe CO lines, a point seized upon by Ayres in favour of his CO cooling hypothesis, claiming that the Carlsson-Stein models could probably be improved through the inclusion of CO cooling, which they lacked entirely. In this respect he was partially incorrect, as in using the Uppsala opacities and equation of state, the Carlsson-Stein model *did* in fact include some CO cooling, though under the ICE approximation whereas that he suggested was via non-equilibrium chemical evolution.

The debate continues however, as evidenced by the statements of Ulmschneider (2003). The author notes his concern at the claims of Ayres and his followers as to the extreme time-dependence of the chromosphere. In another misunderstanding by the Harvard group of the new picture being pushed, Ulmschneider worries that the traditional outward temperature rise of models such as VAL “... should not be discarded prematurely, particularly at great heights in the chromosphere where the kinetic temperature rises to transition layer and coronal values.”. The retention of the traditional temperature rise in the *upper* chromosphere has never been in question by the COmosphere proponents, especially not so high as in the transition region or corona.

Figure 4.5: Time-averaged CO concentration in a strongly dynamic snapshot (during a strong disturbance) of a Carlsson-Stein model, according to the ICE approximation and non-ICE chemical evolution calculations. “Evolution till equilibrium” refers to the CO concentration being allowed to evolve via non-ICE chemical evolution for an indeterminate time between snapshots until equilibrium is reached and the simulation continues. “Saha chemical equilibrium” refers to equilibrium CO concentrations having been determined directly from the Saha relations rather than allowed to find their own equilibrium point. The ICE approximation can be seen to overpredict CO concentrations above 700 km. (Figure taken from Asensio Ramos et al. 2003)



4.3 The Current State of Affairs and The First Study to be Undertaken

Given the growing concern (Uitenbroek 2000a,b; Ayres 2002) over the possible inaccuracy of the ICE approximation, Asensio Ramos et al. (2003) set to investigating departures from ICE in CO lines using the Carlsson-Stein model. They performed non-ICE chemical evolution calculations in radiative transfer simulations used to produce model CO lines from the inherently ICE 1D Carlsson-Stein model atmosphere. The results (Fig. 4.5) indicated that the ICE approximation was in fact perfectly reasonable at disc centre, though overestimated the extension of the off-limb emissions. The first of these findings might seem somewhat surprising given that Uitenbroek (2000a) came to the opposite conclusion modelling CO in the disc, though Asensio Ramos et al. explain this quite plausibly by the fact that the snapshot used by Uitenbroek was from a rather preliminary version of the Stein-Nordlund models that was in fact too cool at the CO line-forming heights. They noted that test calculations using the improved version of the Stein-Nordlund code (Asplund et al. 2000b) to be employed in this study agreed far better with observations than those of Uitenbroek (2000a), though as we demonstrate in Chapter 7 even this version can be improved upon. The results of non-ICE modelling towards the solar disc edge and beyond the limb indicated that significant concentrations of cool CO gas extend just 700 km above the Sun’s surface, in agreement with some observations (e.g. Ayres & Rabin 1996) but slightly lower than the 800-900 km observed by others (e.g. Ayres 2002; Solanki et al. 1994). This of course makes no statement however as to the significant extent of other cool gas at heights greater than 700 km.

The first of the two studies to be undertaken is similar to that of Uitenbroek (2000a), but with an improved 3D model as its basis. The exact method used and its differences with Uitenbroek’s will be quantified in Chapter 7, but the qualitative significance of the

planned differences in the context of the CO debate will be outlined here. Our study differs from that of Uitenbroek (2000a) in a number of significant ways. Firstly, the model used will be the modern hydrodynamical model atmosphere code described in Chapter 3. Secondly, the radiative transfer will be performed over the full range of snapshots of the model atmosphere rather than just one, and the results temporally averaged. Thirdly, the radiative transfer will be calculated over the entire interpolated domain (cf. §3.2), not a 2D vertical slice through it. Fourth, the line profiles produced will be analysed to the point of comparing bisectors with observation, a technique highly sensitive to small deviations of the simulation from reality. Finally and most importantly, the simulations will extend to almost 1Mm above the surface. The first three of these will provide a far more accurate description of CO than the model used by Uitenbroek, and the fourth will enable a more precise evaluation of the reality of the model used in the context of CO. The fifth will allow simulation of line formation in the disputed COMosphere, enabling realistic conclusions to be drawn about its temperature structure.

In particular, the horizontal inhomogeneity admitted by modelling in 3D will allow a variable temperature and therefore height of line formation across the domain. If the derived line profiles agree with observation, the models will thereby indicate a realistic, inhomogeneous temperature structure not possible in 1D analyses. It should be noted that the study will not reproduce the ubiquitous chromospheric emission, as it does not include magnetic fields or extend to great enough heights.

Solar Abundance Measurements

5.1 Abundance Determinations (in any dimension)

By definition, the depth and strength of a spectral line depend upon both the observed continuum level and the observed line intensity. These in turn depend upon continuum absorption and emission as well as line absorption processes. The observed continuum intensity will clearly reflect the amount of continuum-forming species present at various heights, whereas the line intensity will independently reflect the amount of the species responsible for the line. Hence, line depths and strengths depend upon the local ratio (integrated over the path from surface to observer) of the line-forming species with the continuum-forming species. The analysis of line properties can therefore be used to infer an abundance ratio of the two species, under the assumption that abundances are constant at all heights in the solar atmosphere (which is reasonable given the occurrence of convective mixing). In the case of lines in a star, hydrogen is obviously the most abundant species and responsible for the continuum (via H^- in the optical and infrared), so stellar abundances are measured relative to hydrogen. Typically, the abundance ϵ_i of a species i is quoted in logarithmic units of concentration ratio against hydrogen, with hydrogen defined to have $\log \epsilon_H = 12.00$. That is,

$$\log \epsilon_i = 12 + \log\left(\frac{n_i}{n_H}\right) \quad (5.1)$$

where n_i and n_H are local densities of the species in question and hydrogen respectively.

Line strength is the most useful property in determining this ratio for a given species. The strength of weak lines is close to proportional to the abundance of the species responsible for the line, and near proportional to the square root of the abundance for stronger lines (Gray 1992). This arises because in the hotter, lower regions at which weak lines form, their line opacity is dominated by thermal broadening, whereas at greater heights pressure broadening is most significant. The collisional damping factor γ (cf. §2.3.5) is a measure of collision frequency and therefore dependent upon a whole raft of thermodynamic properties, so variable across the atmosphere. Weak lines are preferable to strong ones in abundance analyses, as the strengths of the latter will reflect inaccuracies in γ across the simulation domain. Stronger lines are also more likely to be affected by NLTE and velocity broadening.

An equivalent parameter to abundance in the analysis of line strength is the quantum-mechanical transition probability, or **oscillator strength** f . This is because the dependence of line strength upon f is identical to its dependence upon ϵ_i , such that it is really the factor $f\epsilon_i$ that is dealt with in abundance calculations (Gray 1992). Typically, os-

cillator strength is bundled with the statistical weighting of the lower energy level of the transition g and given as a gf -value. The significance of gf values are that abundance calculations depend very strongly on their being accurate; a large amount of derived or experimentally obtained atomic results exist and obtaining gf values for a line set is not necessarily difficult (though often can be), but it is important. Uncertainties in gf values contribute significantly to error bars in many abundance determinations (Stix 2002).

The general technique for performing an abundance measurement is to synthesise a series of lines using a model atmosphere, allowing $f\epsilon_i$ as a free parameter. By iteratively varying $f\epsilon_i$, the modelled spectral lines are fitted as best as possible to the observed spectrum and the abundance measure thereby computed. This method is illustrated in the profile of Fig. 5.1. Here three different solutions to the radiative transfer problem were computed (green curves) with abundances differing by 0.2 in logarithmic units ('dex'), then interpolated between according to the observed data (blue diamonds) to arrive at the best fit profile (red curve) and its corresponding $\log \epsilon$. Computation of three different profiles and interpolation between them is just one implementation of the general technique known as **curve of growth** analysis. In such an analysis, line strength or shape is in one way or another calculated as a numerical function of abundance, and the abundance best corresponding to the observed shape or strength is chosen. It should be noted at this point that the term 'abundance measurement' is used loosely; abundances are not *measured* but *generated* using a particular model atmosphere. The run of temperature, pressure and density obviously all have a great effect upon line strength too, so abundance measures can only ever be as good as the weakest link in their combination of model atmosphere, gf values and an appropriate line list.

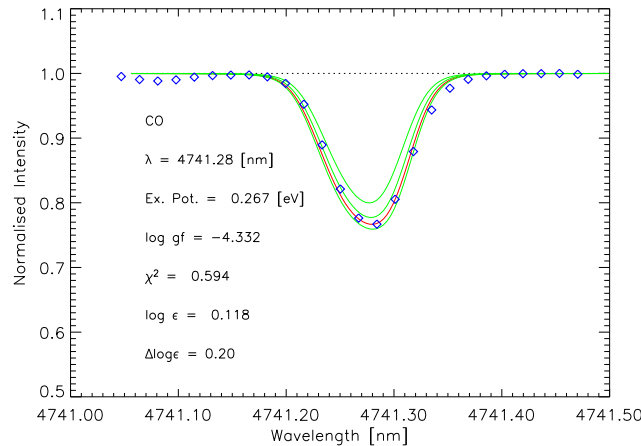


Figure 5.1: An absorption line calculated assuming three different abundances (green lines) differing by 0.2 dex. The three curves were iterated between (red line) in order to produce the best fit to observed ATMOS data (blue diamonds). The logarithmic abundance parameter of this curve is the derived difference from the starting logarithmic abundance. (As will be discussed in Chapter 8, for this case the abundance difference can be interpreted as a change in carbon abundance.)

Two methods exist for determining what constitutes a good fit: **equivalent width fitting** and **profile fitting** (using, for example χ^2 -analysis). Equivalent width fitting simply involves altering $f\epsilon_i$ until the equivalent width of the two lines agrees, whereas profile fitting by χ^2 -analysis requires the minimisation of the χ^2 statistic with $f\epsilon_i$ as the

independent variable. The former has the major advantage of being very simple to perform, and is able to deal with blended lines effectively if all relevant blends are known, given a set of equivalent widths previously measured from observation. Equivalent width fitting can suffer from blends not picked up though, as it has the disadvantage that it ignores profile shape entirely. This does mean though that it has the advantage of being independent of any macroturbulent or instrumental (cf. Chapter 6) profiles; since such convolutions are area preserving, though they might change the shape of the profile they do not alter its strength¹. The latter method is highly accurate thanks to its evaluation of fit with every part of the observed line, though suffers markedly as soon as any blended lines are present unless appropriate parts of the spectrum are masked during the calculation of χ^2 .

Neither method is immune to the influence of microturbulence and other broadening effects that act upon the *opacity* rather than the resultant line profile. In the case of 1D abundance analysis, microturbulence must also enter the calculations and be fitted for. That is, the derived abundances for the lines used are plotted against wavelength, excitation potential and line strength, and any trend sought (e.g. Asplund et al. 2004c; Harris et al. 1987). Microturbulence is iteratively altered in the analysis in an attempt to reduce these trends (cf. the discussion of VAL in §4.1). There is no physical reason why actual abundance should depend upon the line used to measure it, so the existence of a trend is an indication of a physically poor model. The lack of trends is not however necessarily an indicator of a physically realistic one.

5.2 Abundances in 3D: Methods and Effects

The curve of growth analysis for an abundance determination using a Stein-Nordlund model is performed in the manner described for Fig. 5.1 (e.g. Asplund et al. 2000c; Asplund 2004; Asplund et al. 2004c). That is, a number of profiles (typically 3) for the same line are computed using $\log gf$ values in the radiative transfer program differing by a step (typically 0.2 dex) about the known $\log gf$, corresponding to profiles produced by $\log \epsilon_i$ differences of the same amount. As the difference in $\log \epsilon_i$ is very small between profiles, the curve of growth is approximated to be linear in the region between them. That is, the variation of line profile intensity at any given wavelength value between different simulated curves is approximated to be a linear function of $\log \epsilon_i$, so the curves are linearly interpolated between to obtain the line that best fits the observed spectrum. The derived abundance is then just the abundance corresponding to the chosen line, averaged over all lines in an appropriate list. This method allows the choice of either equivalent width or χ^2 fit evaluations, as the curve of growth that has been implicitly derived is not specifically a function of line strength so can be interpreted in terms of either equivalent width or overall profile shape.

The effect of 3D hydrodynamical models over traditional 1D analyses has generally been reduced abundance measurements (e.g. Asplund et al. 2000c; Asplund 2000; Asplund et al. 2004a). Compared to the standard solar composition published by Grevesse & Sauval (1998), the Stein-Nordlund models have derived reduced solar abundances of Fe, Si, C, N and O (Table 5.1). The exact reasons for the decline in abundance in 3D are difficult to quantify given the interdependence of nearly all aspects of the atmospheric description in 3D, though the validity of the models is well established (cf. §3.4).

¹Not theoretically anyway, though in practice they can make a tiny difference, as will be seen in Chapter 8.

Table 5.1: Solar elemental abundances derived using 3D convective models compared to standard values (Grevesse & Sauval 1998). Fe abundance after Asplund et al. (2000c), Si after Asplund (2000), Be after Asplund (2004), C after Asplund et al. (2004a), N after Asplund et al. (2004b) and O, Ne and Ar after Asplund et al. (2004c).

Element	log ϵ	
	Standard	3D
Be	1.40 ± 0.09	1.38 ± 0.09
C	8.52 ± 0.06	8.39 ± 0.05
N	7.92 ± 0.06	7.80 ± 0.04
O	8.83 ± 0.06	8.66 ± 0.05
Ne	8.08 ± 0.06	7.84 ± 0.06
Si	7.55 ± 0.05	7.51 ± 0.04
Ar	6.40 ± 0.06	6.18 ± 0.08
Fe	7.50 ± 0.05	7.45 ± 0.05

In general, the lower abundances appear to occur due to temperature inhomogeneities in 3D, because the temperature dependence of line formation is nonlinear. The lower emergent mean temperature structure in 3D also increases molecule formation and therefore decreases abundances derived from molecular lines.

5.3 C and O Isotopic Abundances and The Second Study to be Undertaken

Early measurements of the solar $^{12}\text{C}/^{13}\text{C}$ ratio using CH lines were typically higher than the currently accepted terrestrial ratio of $92.5^{+7.5}_{-6.5}$ (Rosman & Taylor 1998), and were characterised by large uncertainties (see Harris et al. 1987, for an inventory of early measures). The two most reliable (lowest uncertainty) determinations performed to date utilised CO lines, producing near-terrestrial ratios of 84 ± 9 (Hall 1973) and 84 ± 5 (Harris et al. 1987). The solar $^{16}\text{O}/^{18}\text{O}$ ratio was also measured in these two studies, producing values of more than² 500 and 440 ± 50 respectively. These are similar to the present representative terrestrial ratio of 487^{+36}_{-31} (Rosman & Taylor 1998).

The geological manner of expressing such measurements is in ‘permil’, a deviation in parts per thousand from the terrestrial value, such that

$$\delta^b\text{X} = 1000 \times \left(\frac{(^a\text{X}/^b\text{X})_{\text{sample}}}{(^a\text{X}/^b\text{X})_{\oplus}} - 1 \right) \quad (5.2)$$

where X is the element in question, b refers to its reference isotope and a to the isotope considered. This way of expressing isotopic ratios is problematic, as it depends upon the agreed terrestrial ratios, which are themselves periodically revised as well as given differing values in two recent IUPAC (International Union of Pure and Applied Chemistry) reports (Rosman & Taylor 1998; Coplen et al. 2002). This notation will hence be avoided wherever possible, though it is unfortunately required in the discussion of some studies. In particular, lunar regolith (surface) analyses of the solar wind included in a review by Wiens et al. (2004) show $\delta^{13}\text{C}$ of less than -105 for one study and 30 to -30 for the combined results of others. $\delta^{18}\text{O}$ values tabulated in the same review for direct measurements upon solar wind particles by two different satellites give 110^{+450}_{-250} and 120^{+280}_{-190} . For comparison, the results of Harris et al. (1987) on the same scale imply $\delta^{13}\text{C} = 59^{+67}_{-60}$ and $\delta^{18}\text{O} = 130^{+145}_{-115}$, without inherent error in the scale due to the uncertainty in terrestrial

²Actually 1.06 times the accepted terrestrial ratio at the time, though Hall (1973) does not state exactly what that was or his source for it.

values taken into account. Though small, the fractionation that might occur in the solar wind is still not properly quantified (Wiens et al. 2004), so such results probably say as much about this process as they do about the actual photospheric ratios.

Isotopic ratios, particularly $^{18}\text{O}/^{16}\text{O}$ play an important role in constraining theories of solar system formation. Clayton (2004) suggests a model where the solar system was formed in a supernova starburst triggered by the merger of a dwarf galaxy with our own galaxy. As type II supernovae produce large amounts of ^{18}O but not ^{17}O , this process is claimed to be responsible for the apparently “... anomalously high fraction of ^{18}O ...” relative to other oxygen isotopes in the solar system. This model predicts a correlation between the $^{18}\text{O}/^{16}\text{O}$ and $^{30}\text{Si}/^{28}\text{Si}$ solar ratios, something that will be made easier to test by the more accurate measurement in this thesis of $^{18}\text{O}/^{16}\text{O}$.

Recently, Yurimoto & Kuramoto (2004, see also Yin 2004) have proposed a model of solar system formation whereby oxygen isotopic fractionation occurs in the protosolar cloud due to UV irradiation. The theory predicts that when UV radiation from a source such as nearby stars or even the forming Sun irradiated cool clouds in the protosolar disc, $^{12}\text{C}^{16}\text{O}$ in the outermost layers photodissociated, absorbing all incident radiation around its dissociation energy and thereby shielding the innermost areas from the UV photons. The lower concentration isotopomers $^{12}\text{C}^{18}\text{O}$ and $^{12}\text{C}^{17}\text{O}$ on the other hand, could not absorb all photons around their dissociation energies and therefore did not provide ‘self-shielding’ of the inner regions of the cloud against photodissociation. In this way, the centres of the clouds came to exhibit ^{16}O -rich CO and $^{17,18}\text{O}$ -rich atomic oxygen, which were differentially transported via assorted migratory and molecular means to various parts of the solar system. The upshot of this theory in the context of this thesis is that it predicts a solar $\delta^{18}\text{O}$ of -50, something that can be directly tested with the $^{18}\text{O}/^{16}\text{O}$ measurement to be performed.

The second study to be undertaken as part of this thesis will use appropriate sets of weak $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ lines to rederive solar values of $\log \epsilon_{\text{C}}$, $^{13}\text{C}/^{12}\text{C}$ and $^{18}\text{O}/^{16}\text{O}$. The isotopic ratios will constitute a marked improvement over the 1D analyses of Hall (1973) and Harris et al. (1987), thanks to the use of 3D model atmospheres, more recent gf values, more appropriate line lists and better observations. The determination of the solar carbon abundance using CO lines will provide an important comparison against the soon to be published study of Asplund et al. (2004a) based on [C I], C I, CH and C₂ lines. It will also hopefully circumvent past trouble in using CO lines and 1D models to measure the solar carbon abundance (e.g. Grevesse et al. 1995). In addition to the benefits already mentioned, this study will also provide a better handle on local galactic chemical evolution over the Sun’s lifetime via comparison with the measurements of Langer & Penzias (1993), who measured local ISM $^{13}\text{C}/^{12}\text{C}$ at 62 ± 4 , indicating significant enrichment since the formation of our solar system.

The ATMOS Infrared Solar Spectrum

6.1 The ATMOS experiment

6.1.1 The Instrument

The ATMOS (Atmospheric Trace MOlecule Spectroscopy) instrument is an example of a Fourier transform spectrograph (**FTS**) (Farmer 1994), a class of instruments which produce spectra through the use of a Michelson interferometer. A normal FTS works by recording an interferogram whilst one of its mirrors is gradually moved, altering the optical path difference (**OPD**) between the two arms (Gray 1992). The resulting interferogram hence exhibits various crests and troughs where light of any given frequency periodically interferes both constructively and destructively over the variation in OPD. This interferogram, which exists in the time domain, can then be Fourier transformed to the frequency domain to produce a spectrum of the observed object.

The optical components of the ATMOS instrument are shown in Fig. 6.1. The instrument is a double passed interferometer, meaning that the beam is passed through the interferometer twice before exiting. This is made possible by the use of cat's eye (compound lens) retroreflectors, which offset the split beams and pass them back to different parts of the beamsplitter than the point at which the original incoming beam struck, and the final outgoing beam exits. The section of the beamsplitter where the offset vertical ray strikes is unsurfaced for complete transmission, and the section where the offset horizontal ray strikes is surfaced with gold for perfect reflection (Irion et al. 2002b). Hence, both beams are directed to the retroreflecting mirror at the entrance to the interferometer, are reflected and then retrace their paths back through the apparatus before exiting. The advantage of this double passage over a single pass is that the instrument is far more robust to thermal and mechanical alignment errors (Irion et al. 2002b), and twice the variation in OPD is produced by any given mirror displacement.

The beamsplitter substrate is potassium bromide, and the reflective coating is specially designed for maximum efficiency in the infrared. The Sun is tracked via the use of a double-axis servo controlled suntracker. Unlike a normal FTS, both mirrors of the ATMOS instrument shift simultaneously, providing a maximum OPD of twice their individual 50 cm ranges (i.e. 1 m, with each mirror physically moving 12.5 cm)¹ and a total scan

¹Three factors of 2 define the relationship in this case between maximum OPD and mirror displacement: The standard geometry of reflection, the double passage and the double movement, so that

$$\text{OPD}_{\text{max}} = 12.5 \times 2 \times 2 \times 2 = 100 \text{ cm.}$$

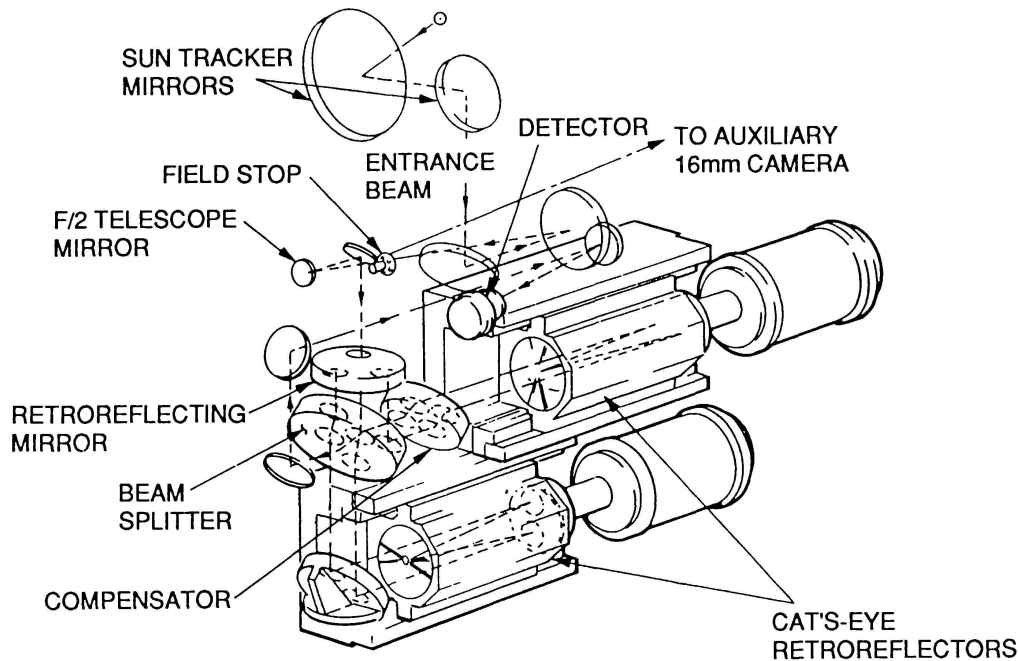


Figure 6.1: The key optical components of the ATMOS FTS. Notice the displacement of the beam caused by the cat's-eye retroreflectors, allowing the instrument to operate in double-passed mode, whereby the beam is reflected off a mirror at the entrance to the interferometer and passed back through the system a second time before exiting. (Figure taken from Farmer 1994)

time of just over 2 s (Irion et al. 2002b). The mirror velocities during a scan are fixed with a 6330Å HeNe reference laser. The interferometer and most auxiliary parts of the instrument are enclosed in an aluminium cover whose internal pressure during operation is kept equilibrated with the surroundings, via a filter designed to keep the interior clean and dry, though which prevented complete evacuation of the instrument even once in orbit. This proved somewhat fortuitous however, as the pressure was low enough to have no effect upon the results except for the detection of absorption lines from trapped H₂O and CO₂, which were used for spectral calibration (Farmer 1994).

6.1.2 Missions

The ATMOS instrument was carried on the SPACELAB-3 (SL-3) and three ATLAS (AT-1,2,3) Space Shuttle flights in 1985, 1992, 1993 and 1994. The primary purpose of the missions was to provide data on the terrestrial atmospheric composition at different heights. This information was obtained by taking absorption spectra of the terrestrial atmosphere at a range of tangent heights from orbit, using the rising or setting Sun as a backlight. On the SL-3 and AT-3 missions however, some measurements were taken well above the extent of the planet's atmosphere as a control for the telluric study, providing as an offshoot a high-resolution infrared solar spectrum free from atmospheric contamination. The SL-3 mission provided a "proof of concept" for the ATMOS study as a whole, recording 4800 pure solar ('high Sun'), spatially averaged, disc centre² interferograms over

²It was suggested (Uitenbroek 2004) that in fact the ATMOS spectrum was not taken quite at disc centre, but integrated over a large central part of the solar disc. If this were the case, then comparative the-

2 days (Abrams et al. 1996). The later AT-3 mission recorded 40 000 interferograms over 10 days, and the resulting time-averaged spectrum is that referred to in this thesis by the term ‘ATMOS solar spectrum’. The major difference in the two missions was an increased signal-to-noise in AT-3 owing to the greater number of spectra, though a great reduction in trapped instrumental lines was also achieved through better purging of the instrument (Abrams et al. 1996).

6.1.3 Data

Following appropriate Fourier transformation of the interferograms, the instrument sampled frequencies from 625 to 4800 cm^{-1} (21 000 - 160 000 Å). This range was split by optical bandpass filters into sections of 625-1500, 1100-2000, 1580-3400, 3100-4800 (SL-3 and AT-3) and 625-2450 (AT-3 only) cm^{-1} (Abrams et al. 1996). The data are available as separate output spectra in these filters, with a resolution of 0.01 cm^{-1} (Farmer 1994). Final averaged spectra were apodized using a medium Beer-Norton function (Farmer 1994; Norton & Beer 1976), discussed in §6.3.2. The AT-3 signal-to-noise ratio varies from 300:1 at the longest wavelengths to 50:1 at the shortest (Abrams et al. 1996). This spectrum is freely available via anonymous FTP at <http://thunder.jpl.nasa.gov/atmos/at3.solar>. A large number of lines have been identified in the ATMOS spectra since its maiden flight (e.g. Geller 1995), with over half attributed to CO.

6.2 ATMOS Data Extraction for the CO Studies

6.2.1 Profiles

Programs were written in Interactive Data Language (IDL) to extract sections of the ATMOS spectrum (`atmos_read` and `spec_read` in §A.1). The data were read from the appropriate filter data file and converted from the ATMOS native data format to an absolute intensity-wavelength format, where wavelength was expressed in nanometres. This was performed according to the scaling instructions of Irion et al. (2002a) using information from the accompanying header file. The spectra were then normalised, with the continuum level defined as the highest intensity point in the extracted section. Given the high signal-to-noise of the data, this was sufficient for continuum determination, as detailed averaging was deemed unnecessary. Using one of a pair of spectral Doppler-shifting routines also written in IDL (`DopplerVtoL` and `DopplerLtoV` in §A.1), the Sun’s gravitational redshift of 633 ms^{-1} was removed from the resulting spectra. An example of an extracted spectrum can be seen in Fig. 6.2.

6.2.2 Bisectors and Line Properties

Further IDL programs were written (`line_analyse`, `obs_line` and `bulk_CO` in §A.1) to calculate, display and store line bisectors from the extracted ATMOS spectrum. Following

oretical profiles would need to be synthesised at some representative μ slightly less than one, or integrated over the appropriate μ values following the radiative transfer simulations. The concern raised appears relevant to the SL-3 flight (e.g. Uitenbroek 2000a,b), though from what little information is available, the AT-3 spectrum on the other hand actually *was* “... nominally disc centre ...” (Abrams et al. 1996, a concept supported by Irion et al. 2002b and Harris et al. 1987). In any case, representative line syntheses were carried out at disc centre and at an average $\mu = 0.91$ implied by the possible ‘worst case scenario’ of integration over a disc of 0.58 $R_{\odot}$ (as reported by Uitenbroek 2000b). Virtually no effect was seen on line bisectors, whilst profile depth and abundance differences were very small (i.e. < 0.02 dex).

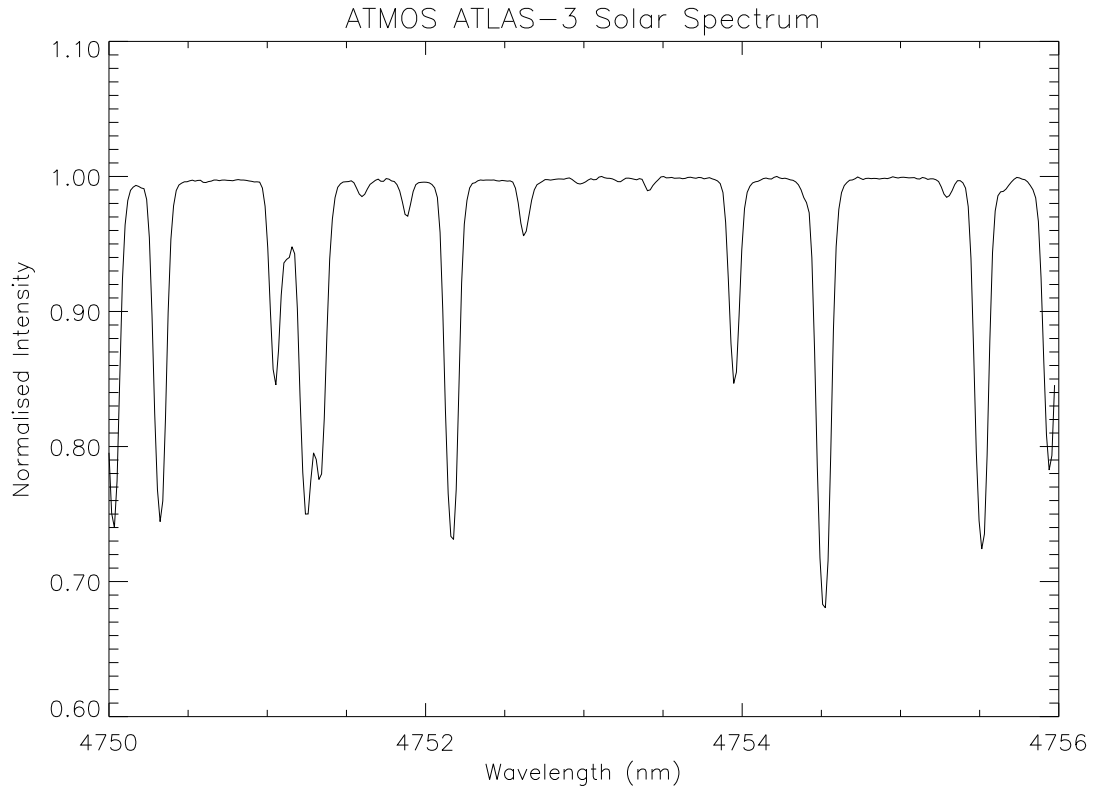


Figure 6.2: An example extracted section of the ATMOS solar spectrum. The feature at 4752.2 nm is a strong CO line used in the analysis of Chapter 7. The other features are not in our line database.

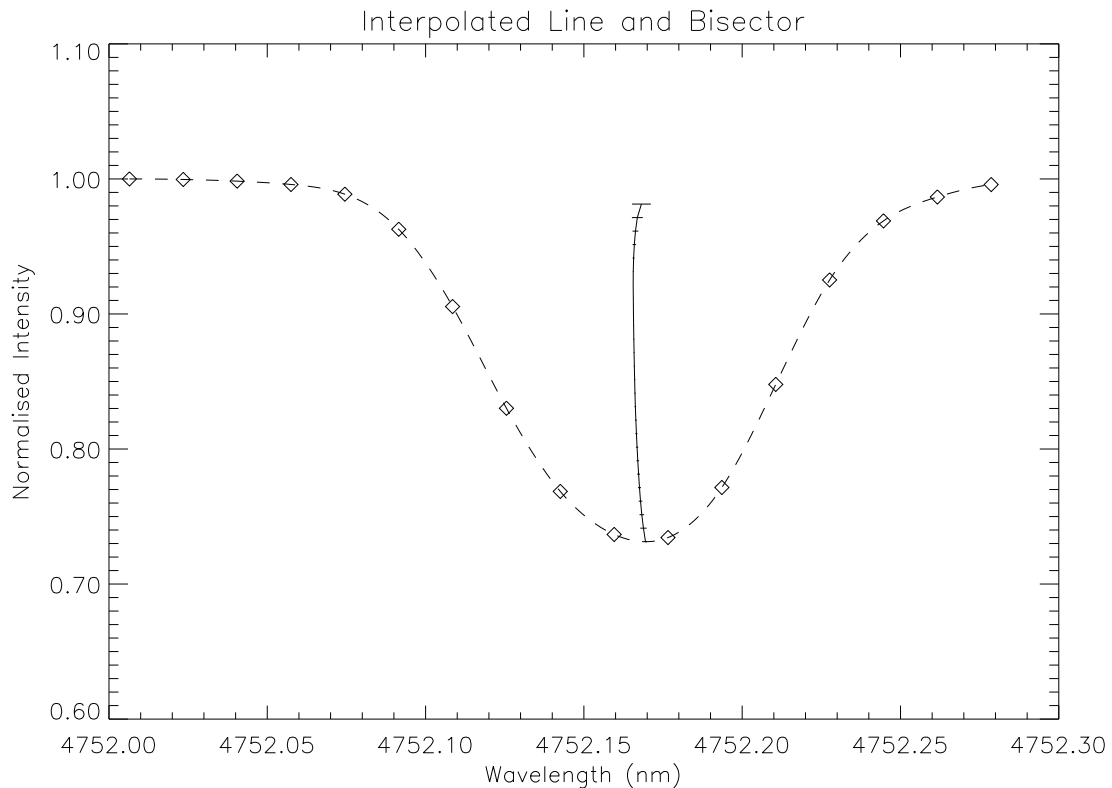


Figure 6.3: An example profile and calculated bisector showing error bars (horizontal ticks) for the same 4752.15 nm CO line identified in Fig. 6.2. The error bars and curvature of the bisector appear small due to the wavelength scale. The observed data points are marked with diamonds and the interpolated profile used for bisector construction is marked with a dashed line.

extraction of a line, it was interpolated to a 0.001 nm resolution wavelength scale. The lowest intensity value in the interpolated profile was taken to be the line depth, and the wavelength corresponding to it the line centre, allowing line shift to be calculated using the Doppler-shift utilities and the laboratory wavelength. The interpolated line was then split in half at its centre and each half separately reinterpolated to a 0.01 resolution (in normalised units) intensity scale before being recombined. The splitting was necessary as the cubic spline method used for both the wavelength and intensity interpolations requires a monotonically increasing abscissa vector, so the use of intensity as abscissa in the second interpolation necessitated the split. Following recombination, the halves of the line possessed data points with common intensities, allowing the average of opposite points' wavelengths to be calculated and a line bisector thereby computed.

Wavelength errors were estimated for each bisector point from the given signal-to-noise of the data, based upon the approximation

$$\delta x = \delta x \frac{\delta y}{\delta y} = \delta y \frac{\delta x}{\delta y} = \delta y \frac{dx}{dy},$$

where $\delta y = \frac{Data}{S/N}$ and S/N is the signal-to-noise at the wavelength of *Data*. S/N was simply fitted analytically to a linear function passing through the two given signal-to-noise values of 50:1 (at 2083 nm) and 300:1 (at 16 666 nm) (Abrams et al. 1996), such that

$$S/N(\lambda) = 0.017143\lambda + 14.29, \quad (6.1)$$

where λ is in nm. In reality, some representative measurements of the noise in quiet parts of the ATMOS spectrum revealed that the S/N values given by the ATMOS investigators were exceedingly conservative estimates, and the true S/N was up to an order of magnitude greater in places. However, for the sake of simplicity, the given S/N was used rather than recalculating it. The section of the bisector above 0.98 normalised intensity was truncated, as closer to the continuum it is dominated by observational noise rather than line asymmetry. An example profile, its interpolated form and bisector showing error bars can be seen in Fig 6.3. Programs were written to perform multiple bisector calculations given a list of lines and a width of extraction from ATMOS about a line centre (`bulk_CO` in §A.1), as well as measure the line strengths with a left-handed Riemann sum and save them along with shifts and depths (`trends` in §A.1).

6.3 Simulation of Instrumental Effects in Model Output

6.3.1 Theoretical FTS Instrumental Profile: The sinc Function

Any instrument is only capable of producing measurements with a finite resolution. In the case of an FTS, the resolution available between two wavelengths (or equivalently, frequencies) is limited by the total OPD available to the instrument. In order to extract enough information to distinguish between two nearby frequencies, an FTS must vary its OPD over a full beat pattern of the pair (Skoog & Leary 1992). Hence, if the FTS maximum OPD is less than one total wavelength of the beat pattern of the pair, the two frequencies cannot be resolved. The length of this single beat pattern for any two light waves is equal to a multiple n of one's wavelength and $n + 1$ cycles of the other's

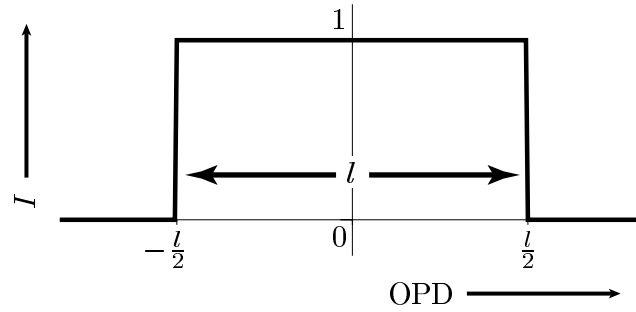


Figure 6.4: The interferometer profile of an ideal FTS: a ‘top-hat’ function. This function is due to the finite range of OPD values samplable by the FTS, owing to its finite maximum mirror displacement. In reality, various instrumental effects tend to produce interferometer profiles somewhat different to a perfect top-hat function.

wavelength, such that the length l is given by

$$\begin{aligned}
 l &= n\lambda_1 = (n+1)\lambda_2 \\
 \Rightarrow \quad n &= \frac{l}{\lambda_1} \\
 \therefore \quad l &= \left(\frac{l}{\lambda_1} + 1\right)\lambda_2,
 \end{aligned}$$

which expressed instead in terms of wavenumbers $k_x = \lambda_x^{-1}$ becomes

$$\begin{aligned}
 l &= \frac{lk_1 + 1}{k_2} \\
 \therefore \quad \frac{1}{l} &= k_2 - k_1 \equiv \Delta k.
 \end{aligned} \tag{6.2}$$

Hence, the smallest wavenumber difference that an FTS can resolve is the inverse of its maximum OPD e.g. in the case of the ATMOS instrument, $(100\text{cm})^{-1} = 0.01 \text{ cm}^{-1}$. This finite resolution is a function of the truncation of all sections of the physical interferogram outside the section where $-l/2 < \text{OPD} < l/2$, akin to its multiplication by a box of unit height and width l (a ‘top-hat’ function), as shown in Fig. 6.4. As multiplication in one domain is equivalent to convolution in the Fourier-transformed domain, this truncation has the effect of convolving the final spectrum with an **instrumental profile** (ILS)³ equal to the Fourier transform of the truncation envelope applied by the FTS instrument. In the case of a perfectly box-shaped interferometer profile of length l , the Fourier transform is a classical **sinc** function $\text{sinc}(\pi kl)$ (Gray 1992), where

$$\text{sinc } x = \begin{cases} \frac{\sin x}{x} & x \neq 0 \\ 1 & x = 0 \end{cases}$$

as shown in Fig. 6.5. Hence, an instrument with resolution Δk has an instrumental profile of $\text{sinc}(\frac{\pi k}{\Delta k})$. The convolution of the resultant spectrum with the ILS serves to ‘smear’ adjacent spectral points by an amount essentially equal to the resolution.

The **resolving power** R of an FTS is the number of statistically independent OPD values available to the FTS at any given frequency. That is, it indicates how many har-

³also known as **instrument function** or **instrumental line shape** (i.e. ILS)

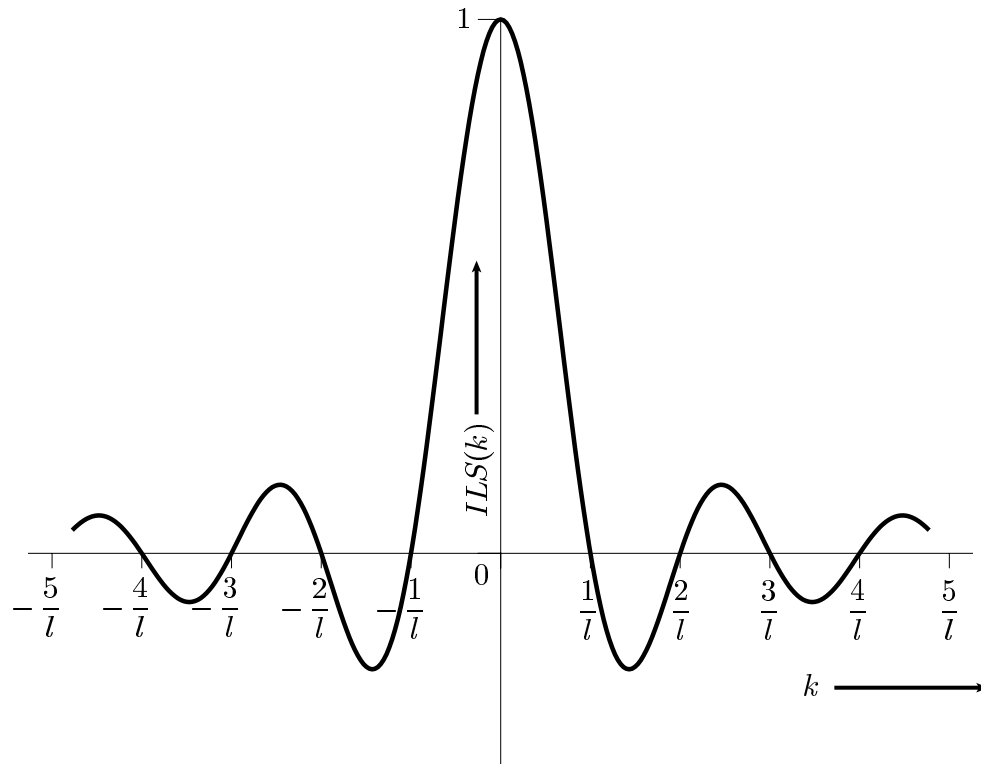


Figure 6.5: The instrumental profile (ILS) of an ideal FTS: a sinc function. This function arises directly from the top-hat of Fig. 6.4, as its Fourier transform. In observing a source with an FTS, this function is naturally convolved with the observed spectrum, smearing adjacent points and giving rise to finite instrumental resolution. In practice, various individual instrumental foibles generally produce an ILS somewhat different to a perfect sinc.

monics of the resolution wavenumber Δk can fit inside a single cycle with wavenumber k , and therefore be distinguished from it. It is hence simply the ratio of the given wavenumber to the resolution. This is not quite the number of different wavenumbers measurable by the FTS in an absolute sense, but the number of linearly independent wavefunctions accessible to the instrument at some given wavenumber. This is a property of the information in the spectrum, and cannot change whether it is expressed in terms of wavenumber, wavelength, frequency or even Doppler velocity from a given reference wavelength. Hence,

$$R = \frac{k}{\Delta k} = \frac{\nu}{\Delta \nu} = \frac{\lambda}{\Delta \lambda} = \frac{c}{v} \quad (6.3)$$

Resolution in wavenumber may therefore be converted to an equivalent minimum discernible wavelength, frequency or velocity difference at some wavelength. Taking a representative wavenumber of 2000 cm^{-1} (corresponding to a wavelength of 5000 nm) for the section of the spectrum predominantly considered in this thesis, the ATMOS instrument's resolving power for our purposes can then be calculated:

$$R = \frac{k}{\Delta k} = \frac{2000}{0.01} = 200\,000$$

Knowing the instrument's resolving power, it becomes possible to simulate the observational effect of an FTS. This is simply done by convolving modelled spectra with an ILS

function characterised by the spectral resolution in the appropriate scale. In the case of the current study, the modelled spectra were expressed in terms of Doppler velocity so the convolving function argument, given by Eq. 6.3 was $\frac{c}{R} = 1.5 \text{ kms}^{-1}$.

6.3.2 Apodization

Unfortunately however, FTS instruments are not always so well behaved as to exhibit perfect top-hat interferogram profiles. This was certainly the case with the ATMOS instrument, whose ILS “... was far from a perfect sinc ...” (Gunson 2004). Various sources of instrumental error, such as the finite size of the entrance and detector fields, generally conspire to produce something other than an ideal top-hat function. The amplitudes close to the maximum and minimum OPD often suffer most (Gray 1992).

To deal with the uncertainty in the true instrumental profiles of transform spectrometers, **apodization** is sometimes employed. The process of apodization involves the multiplication of the interferogram with another profile than the typical top-hat function, such as a Gaussian or simple triangle function, with somewhat tapered edges. This of course has the same effect as convolving the spectral output with an ILS that is the Fourier transform of the **apodizing function** one multiplies the interferogram by. The top-hat function is actually itself an apodizing function in that it at least truncates the interferogram outside $\pm \frac{l}{2}$, even if it doesn’t change anything in between. In the sense of a finite-resolution instrument, it is the unity apodization. Any apodizing function that goes to zero outside $\pm \frac{l}{2}$ hence includes an apodization with a top-hat function in its operation in the same way that the act of multiplication of a number by any other implicitly includes a multiplication by 1. The same is true of the corresponding convolution of the spectrum with a sinc function and the ILS of any such apodizing function; convolution with the ILS of an apodizing function has the same effect as successive convolution with a sinc function and the ILS.

The rounded edges ‘wash-out’ the uncertainty in the interferogram profile by reducing the amplitude of the profile edges where the uncertainties typically lie. For this reason, such an apodization was performed on the ATMOS spectrum before its public release (Gunson 2004). Apodization does however have its dark side. The smearing effect of convolution with a sinc ILS can obviously not be improved by further convolution with other ILS profiles, and any apodization has the effect of further smearing spectral points and degrading resolution. The apodization of the ATMOS spectrum served to alter the instrumental profile from something vaguely resembling a sinc to a far more accurately known function, but at the sacrifice of some spectral resolution. The smooth tapering of an apodizing function to the area where the interferogram is cut off at $\pm \frac{l}{2}$ has the result of reducing the secondary maxima of the corresponding ILS in comparison to a sinc function. This is unfortunately the effect that apodization is most often employed for: Suppressing the prominent side lobes of the sinc function, because they offend the sensibilities of those used to the qualitatively different instrumental artefact evident in spectra produced by a non-Fourier spectrograph. In the emphatic words of Norton & Beer (1976), responsible for arguably the most significant work in the field, in such a case “There is, of course, no need to apodize at all.”

The ATMOS spectrum was apodized using a medium Beer-Norton function (Farmer 1994; Gunson 2004). This is one of three functions purposefully created by Norton & Beer (1976) for their minimal resolutional broadening of spectral points and maximal damping of secondary maxima. The three functions as well as the usual sinc function are plotted in

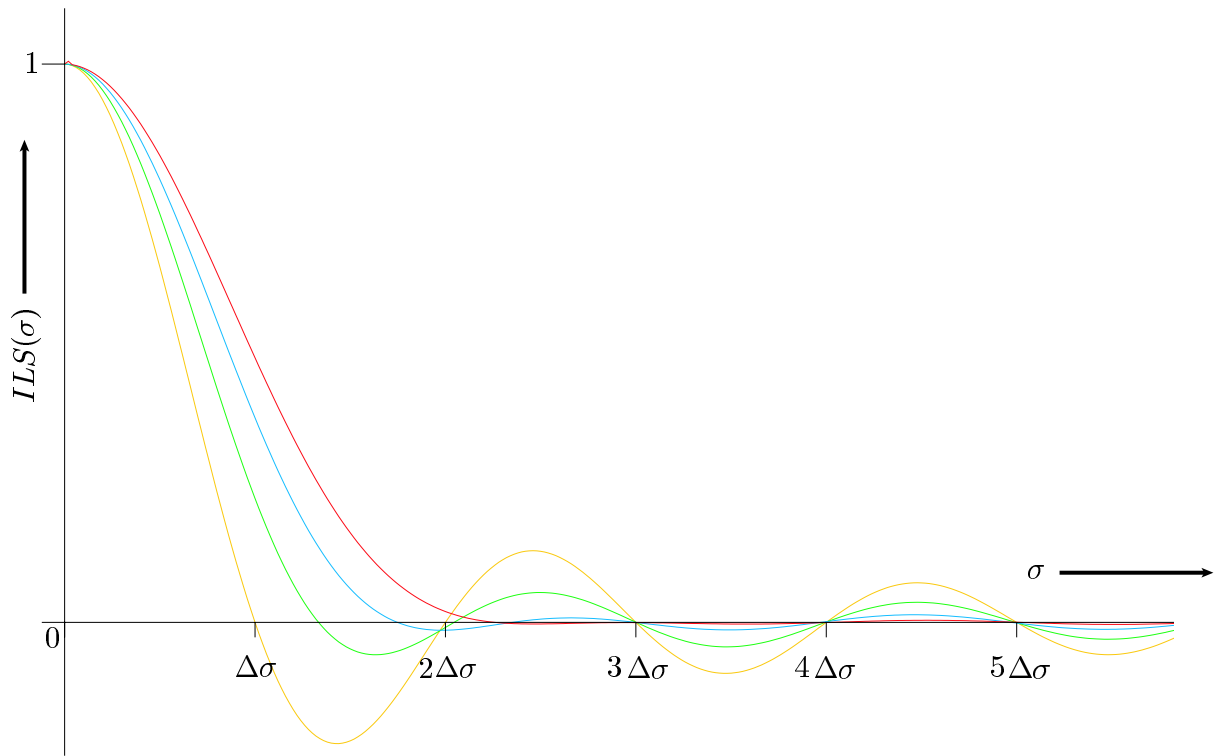


Figure 6.6: ILS corresponding to weak (green), medium (blue) and strong (red) Beer-Norton apodizing functions. The classical sinc function (no apodization) is shown also (yellow) for comparison. Note the decrease in secondary maxima and minima, as well as increase in central lobe width (and therefore resolutional smearing) produced by the apodizing functions over the classical sinc. The Beer-Norton functions are conjecturalised (Norton & Beer 1976) to produce very close to the optimal possible secondary damping for the central broadening they each cause. Note also the trade off between secondary damping and resolutional degradation with increasing strength of apodizing function.

Fig. 6.6, demonstrating the progressive trade-off between damping and spectral integrity, as the secondary maxima can be seen to decrease in height but the central lobe increase in width with increasing strength of Beer-Norton apodization (BNA).

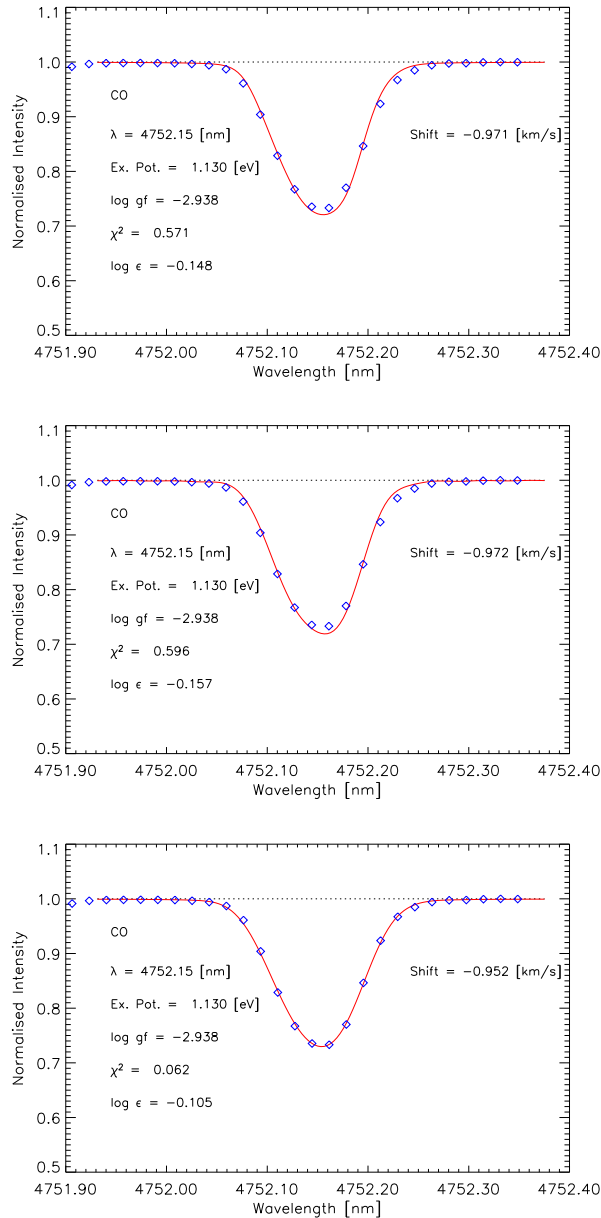
In order to properly simulate the effects of the ATMOS instrument and the post-processing performed by its operators, a program to perform BNA of the model data was written (`beerbroad` in §A.1). Given a line profile and corresponding spectral resolution in any of the units of Eq. 6.3, the program would generate the desired apodizing ILS (weak, medium, strong or classical sinc) and convolve with it. In reflection of the ATMOS data, the modelled profiles to be described in Chapters 7 and 8 were convolved with the ILS of a medium Beer-Norton function⁴,

$$\begin{aligned}
 ILS(\sigma) = & 0.26\text{sinc } a - 0.154838 \frac{3(\text{sinc } a - \cos a)}{a^2} + \\
 & + 0.894838 \frac{-15[(1 - 3/a^2)\text{sinc } a + (3/a^2)\cos a]}{a^2}, \quad (6.4)
 \end{aligned}$$

⁴Reproduced here as much for interest's sake as the fact that the original paper (Norton & Beer 1976) is not easy to come by nor the apodizing functions yet spotted reproduced elsewhere.

where $a = \frac{\pi\sigma}{\Delta\sigma}$, σ is the spectral variable and $\Delta\sigma$ its resolution. As previously mentioned, the spectra σ were expressed in Doppler velocity units and the argument $\Delta\sigma = 1.5 \text{ kms}^{-1}$ based upon Eq. 6.3 used. Carrying out the apodization procedure on our old friend the CO 4752.2 nm line (Fig. 6.7) clearly improves agreement with the ATMOS observations.

Figure 6.7: The effects of the BNA used in Chapters 7 and 8 upon the same 4752.2 nm CO line shown in Figs. 6.2 and 6.3. The profile in the upper panel has had no instrumental profile applied to it, the middle panel shows the profile convolved with a sinc function of $\Delta\sigma = 1.5 \text{ kms}^{-1}$, and the lower panel illustrates the effects of medium BNA characterised by $\Delta\sigma = 1.5 \text{ kms}^{-1}$. Note the excellent agreement between theory and observation in the lower but neither of the other two panels, vividly demonstrating the importance of correctly emulating instrumental effects when working with the ATMOS spectrum.



CO Line Shapes and Asymmetries

In order to use a model to draw accurate conclusions about the temperature structure of the solar atmosphere and the distribution of CO within it, synthesised CO lines must demonstrate excellent agreement with observation. Despite its prior successes, the model described in Chapter 3 must hence be put to the test and found sufficient before its inferences regarding the true nature of CO temperature and location are heeded. To this end, the following study became an iterative one, where the model performance was tested against ATMOS data and some lesser findings made (§7.1), its shortcomings approximately identified (§7.2) and sufficiently remedied to allow accurate remodelling of data before final inferences were drawn (§7.3).

7.1 Phase 1: Initial Comparisons

7.1.1 3D Models

The hydrodynamical simulation used was that described in §3.1. Specifically, it covered a physical area $6 \times 6 \times 3.8$ Mm of which about 1 Mm was above the solar surface, at a resolution of $200 \times 200 \times 82$. The horizontal boundaries were periodic, the lower boundary transmitting and the upper an extended transmitting boundary across which the density gradient was kept hydrostatic. The MHD equation of state and Uppsala opacities were used. Molecular opacities were determined under the ICE approximation, and the entire simulation under the assumption of LTE. Continuous opacities were calculated using opacity binning. Ninety-nine snapshots of the convective simulation were stored, representing just under an hour of real solar time. The model included no free parameters, and was characterised as solar by the accepted gravity, effective temperature and standard solar composition of Grevesse & Sauval (1998). A numerical viscosity was employed to stabilise the simulation. This particular atmosphere was generated in 1999 by Martin Asplund, and is the same atmosphere used in the studies of Fe, Si, O, Be, C and N described in §3.4.

For this study, the 1999 model atmosphere was interpolated to a $50 \times 50 \times 82$ grid extending over the entire original horizontal domain and from approximately 0.7 Mm below to 1.0 Mm above the solar surface. Using the Uppsala package, lookup tables of temperature, density and opacity were generated for each line studied (Table B.1) under the assumption of ICE. As described in §3.2, the three-dimensional radiative transfer equation was solved at each point in the horizontal grid. This was performed for all ninety-nine snapshots and assuming LTE. The standard solar composition of Grevesse & Sauval (1998) was assumed for both table generation and radiative transfer. For each line, the radiative transfer was solved at 141 wavelength points differing by a Doppler velocity of

0.2 kms^{-1} . Profiles corresponding to three abundances differing by 0.2 dex were calculated for purposes described in §7.1.3. The spectra were spatially and temporally averaged, and compared to the ATMOS data.

7.1.2 Line List

The CO lines considered in this study are shown in Table B.1. The line list was provided by Grevesse & Sauval (2004), with the 31 $^{12}\text{C}^{16}\text{O}$ lines specifically selected for use in this study. They are all strong lines, formed high in the atmosphere and therefore ideal for the study of convective motion induced shapes and asymmetries. As the height of their formation and hence the velocity signatures they exhibit strongly depend on the temperature structure of the atmosphere, they are perfectly suited to probing the disputed COMosphere region. The approximate formation heights of these and other line lists used in the second study are shown in Fig. 8.1. The lines were also selected to be free of contamination by blending with other lines.

7.1.3 Post-Processing

The spatially and temporally averaged intensity spectra output by the radiative transfer program were post-processed for display and analysis along with the ATMOS data, using an existing IDL program extensively rewritten for the purposes of this and the following study (`multiprofile` in §A.2). The modelled profiles were apodized with a medium Beer-Norton function of characteristic resolution 1.5 kms^{-1} (cf. §6.3.2), and bisectors of the modelled lines produced. The extracted ATMOS bisectors, profiles and uncertainties (cf. §6.2) were displayed with and compared to the model output via the calculation of a reduced χ^2 statistic. Based upon the standard technique of minimising this measure, the modelled line shift and abundance (using the three different profiles computed for each line) were allowed to vary for best agreement with observation. This fitting was permitted to allow for the possibility of systematic error in the laboratory wavelengths of the lines considered, and the fact that the standard abundances of Grevesse & Sauval (1998) are likely to be too high (cf. §5.2). Unless otherwise indicated, all lines in both this and the following chapter have been fitted in this manner.

Because permitting a variable abundance changes the modelled line strength and depth, the misgivings about absolute abundance and wavelength scale mean that observed line strength, depth and shift cannot be directly compared with their unfitted modelled values as a test of model accuracy. However, because the line shapes and asymmetries of the line list used in this study are what strongly reflect the temperature structure (cf. 7.1.1), the bisectors and line profile shapes are the primary focus of the ensuing analysis anyway, while the other properties play only a supporting role. The comparison of observed and modelled profile depths, strengths or shifts *after* fitting serves as an indication more of the model's accuracy in reproducing the line *shapes* and *asymmetries* than the properties themselves, seeing as the χ^2 fit is based upon the profile *shape*. In essence, if such a delicate measure as the bisectors can be gotten right for such a touchy species as CO, then given the past successes of the model the other properties should fall into line. If anything at all, in such a case the values of these properties *before* fitting should indicate approximate systematic errors in the standard abundances and wavelengths.

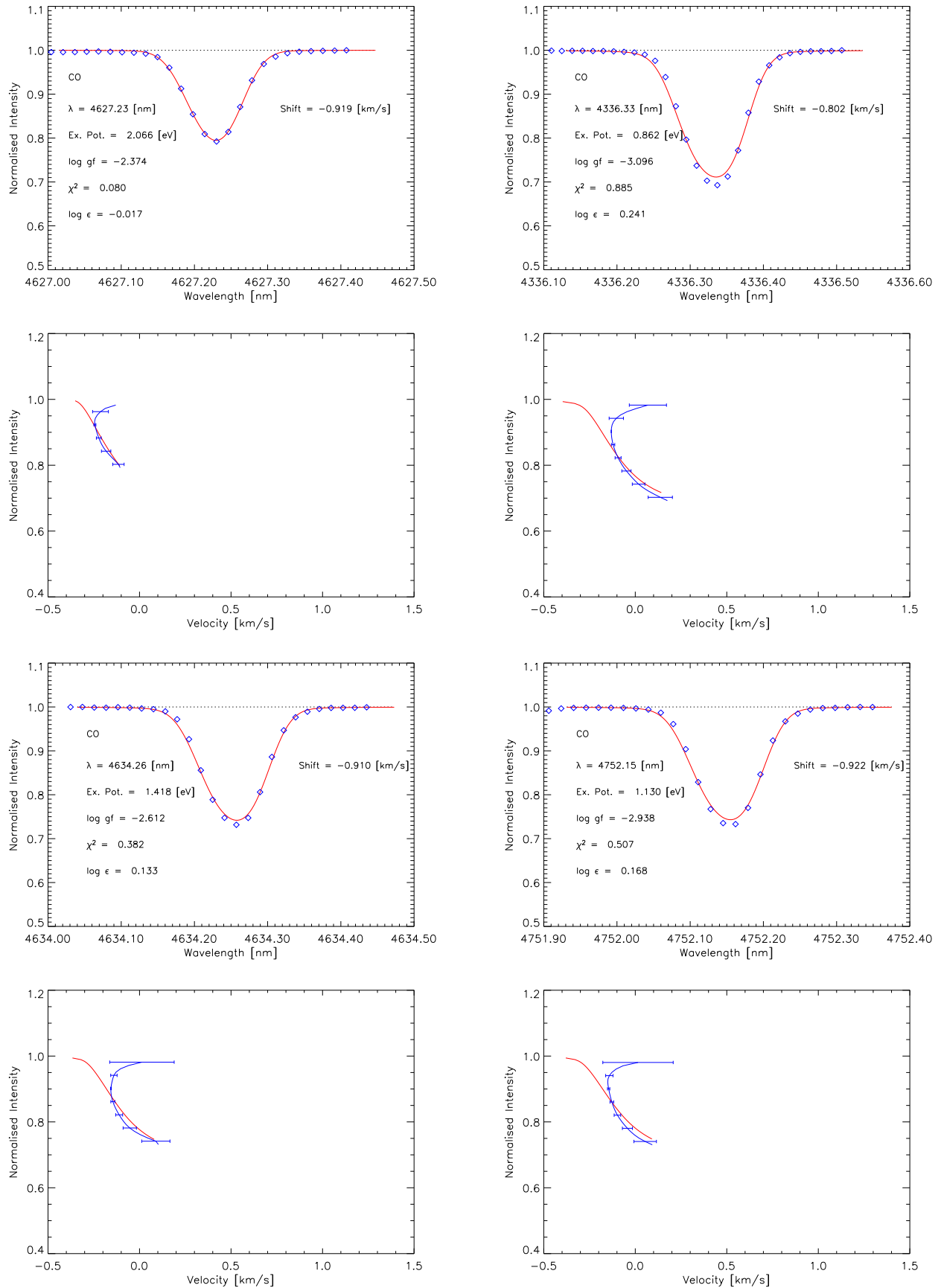
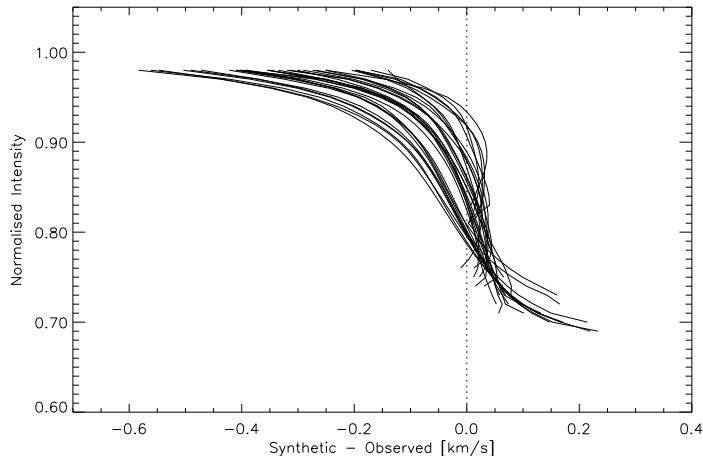


Figure 7.1: Example spatially and temporally averaged, disc centre synthesised CO line profiles and bisectors (red lines). Profiles were calculated using the Phase 1 model, and are compared with ATMOS profiles and bisectors (blue diamonds). The solar gravitational redshift was removed from the observed spectrum, and the theoretical profiles were apodized and fitted in abundance and Doppler shift (see text). The profile agreement is not terrible, but the bisectors are clearly the wrong shape.

Figure 7.2: Differences between observed and synthetic bisectors generated with the Phase 1 model for all 31 lines. The solar gravitational redshift has been subtracted from observations and the synthetic profiles have been apodized and fitted in abundance and Doppler shift (see text). A clear and consistent discrepancy can be seen in the upper halves of each curve, indicating the incorrect shape of the theoretical bisectors.



7.1.4 Results

Profiles were simulated for all 31 lines, apodized and fitted. Some example resultant profiles and bisectors are shown in comparison to their ATMOS counterparts in Fig. 7.1. The differences between the synthetic and observed bisectors for all 31 lines are plotted in Fig. 7.2. Unfitted line shifts of the observed and synthesised profiles as well as their differences are illustrated in Fig. 7.3. The approximate computational time for each synthetic line was half an hour on a 1.2 GHz Sun-Fire-280R with 4 GB of RAM. The average reduced χ^2 value for the agreement between observed and theoretical profiles is 1.087 (standard deviation 1.082). It should be noted that the reduced χ^2 values calculated in both this and the following study are somewhat skewed towards lower values by the points in the continuum, which are always in good agreement¹. They are also heavily skewed towards lower values by the conservative estimate of ATMOS S/N , discussed in §6.2.2. As such, they are useful more as a comparative measure than in an absolute sense, e.g. for use in fitting, or comparing the different versions of the hydrodynamic model described in §7.2 and §7.3.

7.1.5 Discussion

Aside from even considering the modelled profiles and bisectors, it is plain that the observed ATMOS bisectors do not agree with those produced by Blomme et al. (1994), a significant finding in itself. The reason for this discrepancy appears to simply be that Blomme et al. (1994) extended their bisectors only to intensities of about 0.94 of the continuum intensity, whereas those of Fig. 7.1 extend to intensities of 0.98. Given that the bisectors of Blomme et al. (1994) were taken from the more noisy SL-3 flight of the ATMOS instrument rather than the AT-3 flight, this lesser extension is not surprising. Also, seeing as the current continuum was taken as the highest intensity value in the extracted section of the spectrum (cf. §6.2.1) whilst Blomme et al. (1994) no doubt use an averaged continuum, it is also quite likely their determined continuum level was slightly lower than that of the current study. This would then put the bisector cut-off height of the earlier study at even less than 0.94 on the normalised intensity scale of Fig. 7.1.

¹For the same reason, two lines (4666.9 nm and 4584.3 nm) where the section of the ATMOS spectrum compared exhibits parts of other lines (not blends, but nearby lines) are excluded from the average χ^2 value.

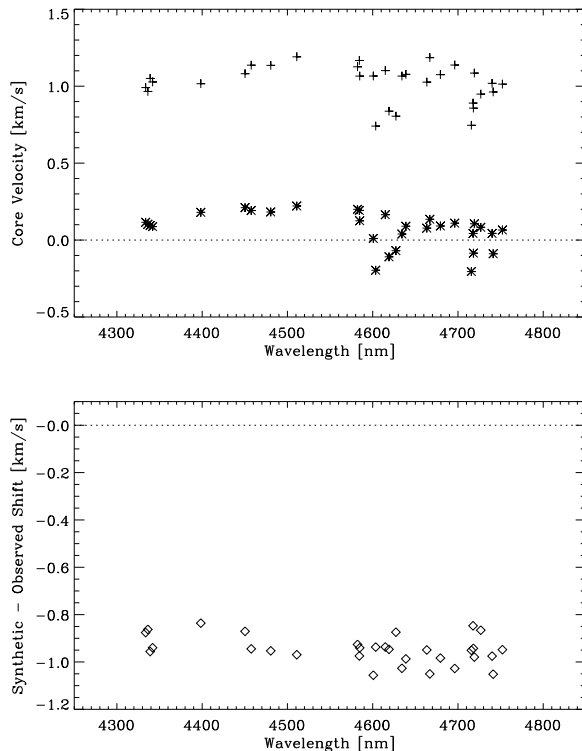


Figure 7.3: *Top:* Unfitted line core shifts in the observed (+) and Phase 1 modelled lines (*). Observed profiles appear very strongly redshifted, suggesting a probable error in laboratory or ATMOS wavelengths. *Bottom:* Difference between observed and modelled shifts, illustrating the approximate likely systematic error in laboratory wavelengths or ATMOS wavelength calibration. However, given the discrepancies seen in Figs. 7.1 and 7.2 this indication should not necessarily be considered accurate.

The modelled bisectors are clearly not in very good agreement with the ATMOS data, worst of all in the regions near the continuum (Fig. 7.2). As was explained in §3.3.1, the blueward tilted shapes are mainly characteristic of absorption occurring very high in upflowing sections of the atmosphere. The ‘curving back’ of the extracted ATMOS bisectors near to the continuum indicate that the strong CO lines may not in fact be entirely dominated by upflows as suggested by the previous study and the Phase 1 model, but that CO present in the downflows possibly contributes a small but significant amount also. If this is the case, then the bisector discrepancy may indicate that the model underpredicts the contribution of the intergranular lanes to the strong lines, pointing at either too low a CO concentration or too slow a velocity field in these regions. Another explanation could just be that the lines form slightly lower in the atmosphere than predicted by the model atmosphere. If this is the case, then the temperature structure of the model atmosphere is likely too high near the top of the photosphere, pushing the strong CO line-forming region outwards. Phase 2 of this investigation is the pursuit of these hunches.

The observed wavelength shifts in the ATMOS data are vastly different from those seen in the model output. The modelled shifts are very close to zero, consistent with the notion that the lines considered are formed high in the atmosphere where velocities are predominantly horizontal. Indeed, such a redshift as demonstrated by the observed lines in Fig. 7.3 is simply too high to have possibly been caused by convective velocities² (Stein & Nordlund 1998; Asplund et al. 2000a). The theoretical-observational discrepancy illustrated in the lower plot of Fig. 7.3 can therefore certainly be taken to indicate some sort of systematic error in the CO laboratory wavelengths or ATMOS frequency calibration. However, proper description of the line shapes and asymmetries must be achieved before

²unless it were exclusively in downflows very low in the atmosphere, which is exceedingly unlikely given the line strength and the fact that the granules cover most of the solar surface.

the discrepancy can be confidently used as a quantitative estimator of this systematic error.

7.2 Phase 2: Tinkering

7.2.1 Altered Atmospheres

In an attempt to identify the deficiencies in the Phase 1 model, a series of altered atmospheres was created from it. Using existing IDL model atmosphere manipulation software, the interpolated Phase 1 model was physically altered in 20 different ways, listed in Table 7.1. Each of the 20 new interpolated model atmospheres had the same radiative transfer simulations run on them as were performed on the Phase 1 model. Not all lines were considered for all models however, as often it could be plainly seen from a small number of lines that an altered model did not improve the CO line bisectors.

7.2.2 Results

The v16 model was a clear-cut winner in the bisector stakes, producing curves reasonably closely matched to the ATMOS data. Models v7 through v15 all changed bisectors to a $\subset$ shape, though none reproduced the ATMOS data so well as v16. Model v18 in particular is noteworthy for having done this also, seeing as it was characterised by the opposite action on the upflows as was variously performed on the downflows in models v7-16. Most notably though, the bisector and line shapes produced with model v18 and its ‘component’ models v19 and v20 were not of as similar a shape to the observed data as those based upon altering downflows, and were clearly not going to be made so by fine-tuning the parameter magnitudes. The model based on an overall temperature decrease (v3) helped curve bisectors backwards, but not quite back in the redwards direction, and grossly overestimated line strength and depth. Model v16 was hence selected for further analysis.

The same example profiles and bisectors as were shown for Phase 1, now recalculated with model v16, are shown in comparison with their ATMOS counterparts in Fig. 7.4. Bisector differences for all 31 lines are plotted in Fig. 7.5, showing a significant improvement over the Phase 1 equivalent plot (Fig. 7.2). Using this model, the average reduced χ^2 value for the agreement between observed and theoretical profiles is 0.967 (standard deviation 0.977)³, also a little better than that achieved in Phase 1.

7.2.3 Discussion

The results of this phase tell us much about the location of CO line formation in the upper atmosphere and the reasons for the inability of the Phase 1 model to properly describe it. There appears not to be quite enough velocity contrast between the upflowing and downflowing regions in the Phase 1 model, indicated by the varying successes of the v7-16 and v18 models. These models also indicate a slight overprediction of temperature in the intergranular areas. A general overprediction of temperature throughout the atmosphere, causing line formation to move outwards cannot be entirely responsible for the discrepancy, as evidenced by the results of model v3. The fact that v16 and its precursors

³As discussed in §7.1.4, χ^2 values are unusually low and only useful for comparative purposes, due to the overprediction of errors in the ATMOS data as well as the influence of the continuum on the fit.

Model	Alterations from Phase 1
v1	Original
v2	All velocities $\times 1.5$
v3	$T + 500K$
v4	$T - 500K$
v5	Density $\times 1.5$
v6	Density $\times 0.75$
v7	Vertical velocities $\times 1.5$
v8	Downwards velocities $\times 1.5$
v9	Downwards velocities $\times 1.3$
v10	Downwards velocities $\times 1.3$, $T - 100K$
v11	Downwards velocities $\times 1.3$, density $\times 0.75$
v12	Downwards velocities $\times 1.2$
v13	$T \times 0.95$ in downflows only
v14	Downwards velocities $\times 1.3$, $T \times 0.95$ in downflows only
v15	Downwards velocities $\times 1.3$, $T \times 0.97$ in downflows only
v16	Downwards velocities $\times 1.25$, $T \times 0.96$ in downflows only
v17	Downwards velocities $\times 0.75$, $T \times 1.04$ in downflows only
v18	Upwards velocities $\times 0.75$, $T \times 1.04$ in upflows only
v19	Upwards velocities $\times 0.8$
v20	$T \times 1.05$ in upflows only
v21	Downwards velocities $\times 0.7$, $T \times 1.06$ in downflows only

Table 7.1: Characteristics of atmospheres physically altered in Phase 2. Model v16 was found to improve bisector shape most.

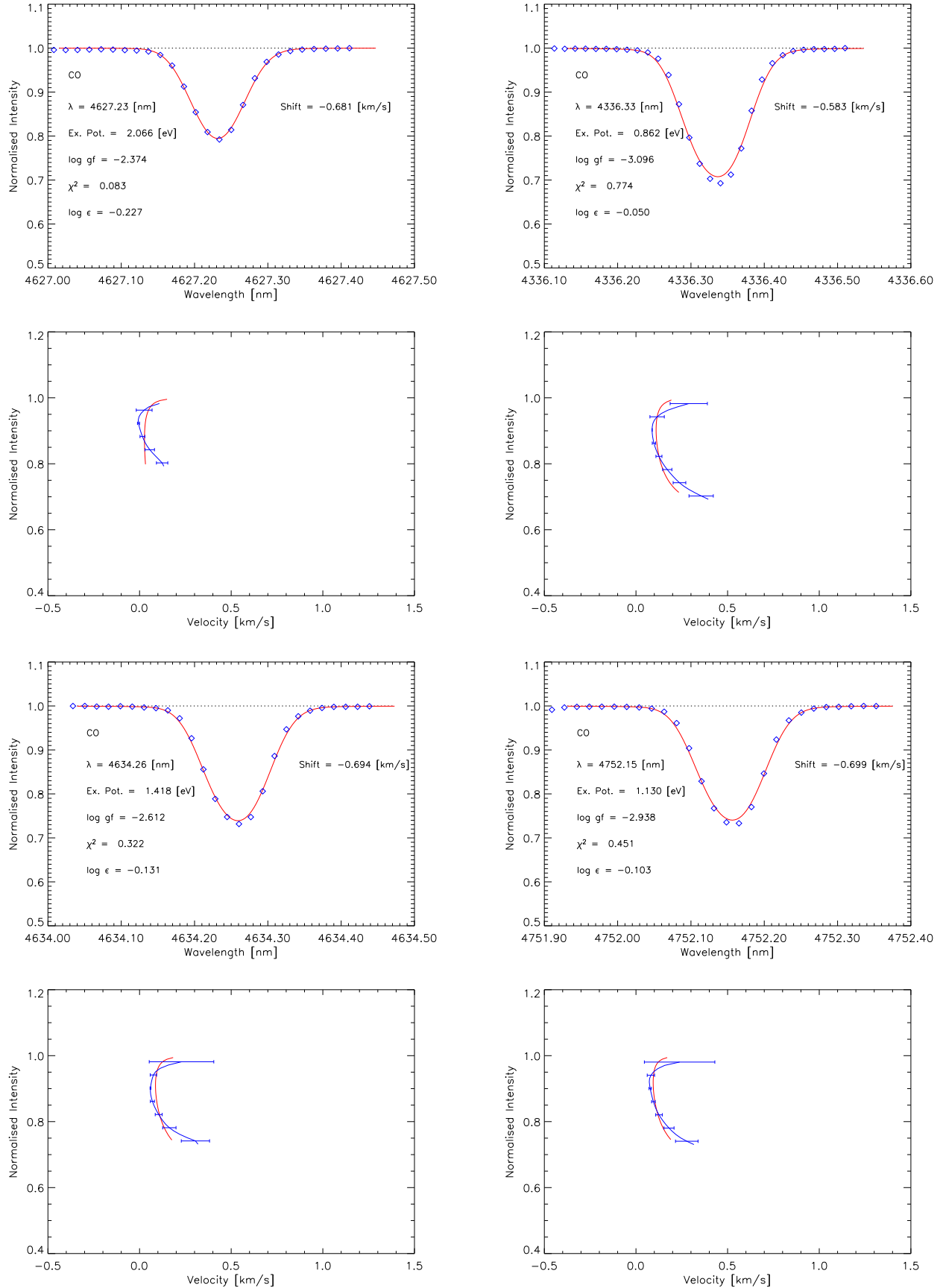


Figure 7.4: The same as Fig. 7.1 but using the Phase 2-v16 altered model atmosphere. The profile and bisector agreement is clearly improved over the Phase 1 results.

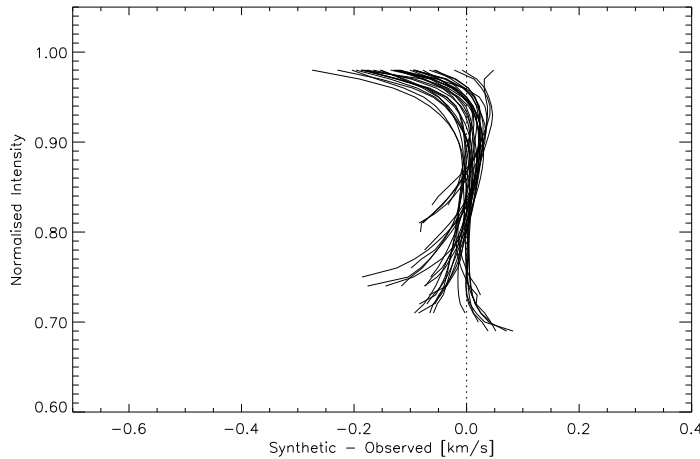


Figure 7.5: Differences between observed and synthetic bisectors generated with the Phase 2-v16 model for all 31 lines. In comparison to Fig. 7.2, the large discrepancy in the upper parts of the bisectors is drastically reduced, reflecting the ‘turning-back’ of bisector tops by the altered model.

performed better than v18 suggests that the deficiency exists in the model’s description of downflowing regions rather than upflows.

Hence, it appears that the upper regions of the intergranular lanes contribute slightly to the strong CO absorption lines in reality, but not in the Phase 1 model. This seems to be because the model overpredicts temperatures in the intergranular lanes, both reducing CO concentration in these areas and increasing the buoyancy of the gas, causing reduced downflowing velocities. In turn, this overprediction of lane temperatures probably shifts line formation slightly outwards and further contributes to the less than perfect description of the line bisectors.

The manual alterations to the Phase 1 model atmosphere performed here must be understood to be completely unphysical. They were arbitrary alterations of whole fields of variables based upon empirical guesses, and as such result in wildly self-*inconsistent* model atmospheres. In reality, any of the changes made would result in feedback upon every other thermodynamic variable at virtually every place in the atmosphere. The models are not presented as alternative descriptions of the reality of the solar atmosphere, but utilised merely as tools for constraining the possible problem(s) with the existing model. Phase 3 deals with true physical improvements attempted on the Phase 1 model subsequent to these findings.

7.3 Phase 3: Improved Models

7.3.1 Improved 3D Model

The ad-hoc test models and subsequent CO line calculations presented in §7.2, suggested that perhaps the error in the Phase 1 model had its source in the upper boundary condition applied to the hydrodynamic simulation. Recalling §3.1.3, the uppermost layer has its velocity structure held constant, density gradient hydrostatic and uppermost energy spatially constant. Seeing as the CO lines were forming in such high layers, perhaps the incoming gas from the uppermost layer may not have had time to properly cool and equilibrate to its surroundings in the intergranular regions by the time it reached CO line formation heights. To test this hypothesis, despite the questionable nature of the equation of state, LTE approximation and ICE treatment at the low densities of such high layers, an attempt to extend the model atmosphere beyond 1 Mm was undertaken.

Following considerable computational difficulty, the new model atmosphere simulations

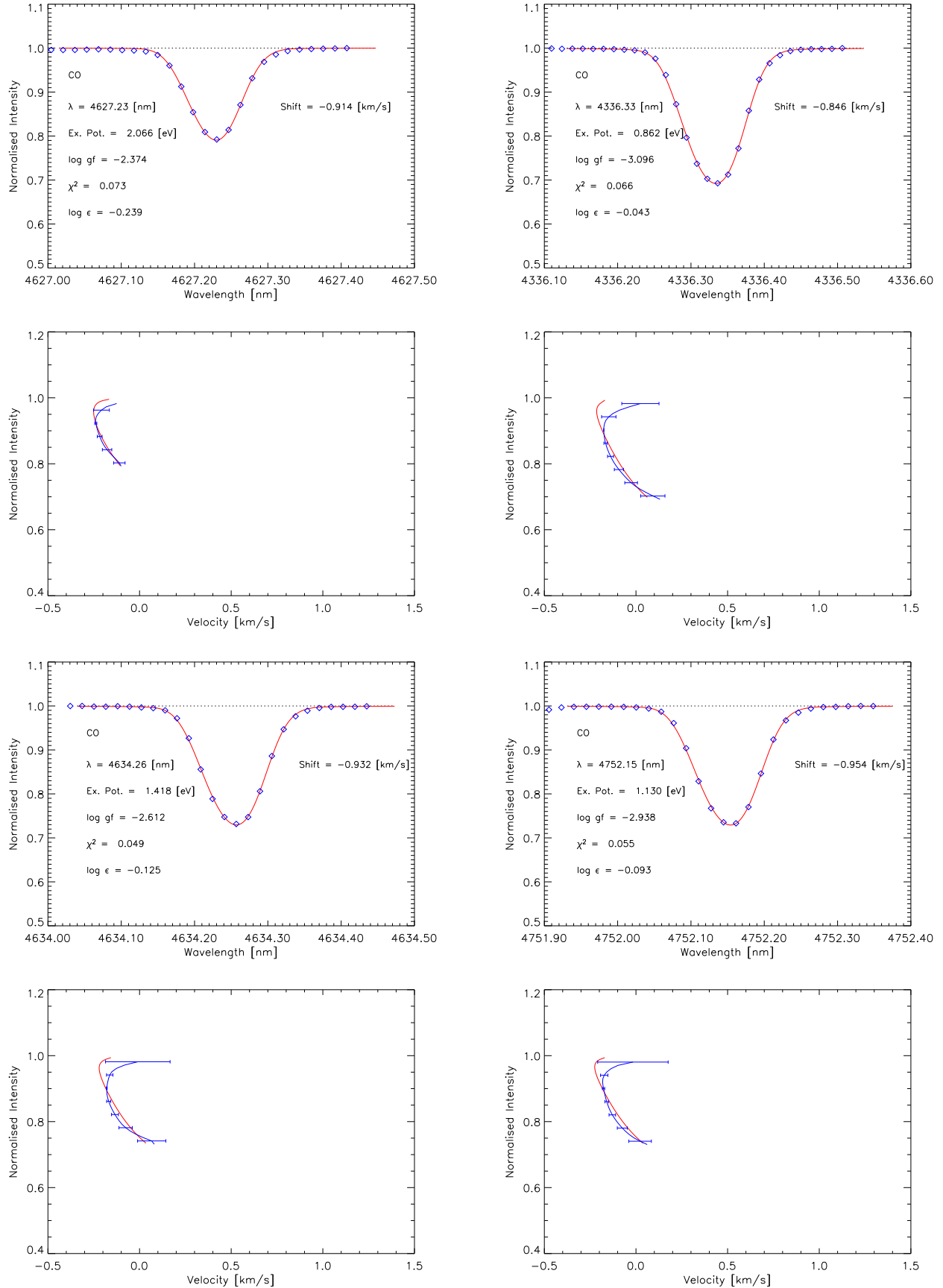


Figure 7.6: The same as Fig. 7.1 but using the standard extension, standard boundary Phase 3-82 improved model atmosphere. The profile and bisector agreement are excellent and very good respectively; both clearly show better agreement with observation than those of either Phase 1 or 2.

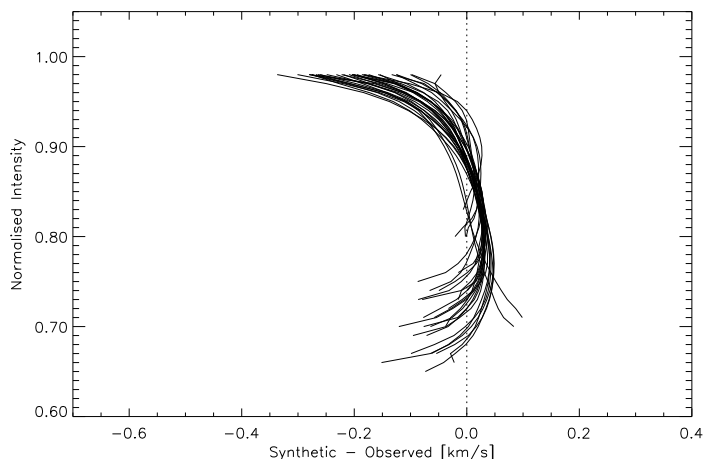
were run and completed. Four new atmospheres were produced, two with the original extent and two extending to heights of almost 1.2 Mm. The extended simulations were run at a resolution of $50 \times 50 \times 88$ and those with the original extension at $50 \times 50 \times 82$. The lower resolution was chosen over the $200 \times 200 \times 82$ of the Phase 1 model due to computational time constraints. This was despite the findings of Asplund et al. (2000a) that not all simulation properties are converged at such resolution, as the new model atmospheres were intended only for qualitative testing of the boundary equilibration hypothesis. The purpose was not to produce the most accurate description of the solar atmosphere available, nor could it be given the questionable validity of the model assumptions at heights above 1 Mm. The $50 \times 50 \times 82$ models served as a control sample for the drop in resolution, and it was anticipated that they would resemble the Phase 1 model.

Two models were run at each resolution so that a new energy condition could be applied to the upper boundary, with one model at each resolution having the original boundary condition and the other the new condition, again providing control samples. It was felt that the existing energy condition could cause extreme horizontal temperature fluctuations across the top layer in the $50 \times 50 \times 88$ case, due to the response of the equation of state at such low densities. In order to avoid this, the flat *horizontal* energy gradient at the top of the domain was replaced by a zero *vertical* energy gradient across the top layer, where horizontal inhomogeneity was permitted. For ease of reference, the original height atmospheres will be designated ‘82’, the taller ones ‘88’ and those with the new boundary condition by an ‘e’, so that e.g. the ‘Phase 3-82e’ model atmosphere is the non-extended version with the new boundary condition, whereas that with the original boundary is the ‘Phase 3-82’ model.

Given that the Phase 1 model atmosphere was generated in 1999, the hydrodynamical simulations have undergone some slight improvements since its creation. These improvements were expected to cause only minor differences in the output atmosphere, especially given the previous successes of the Phase 1 model (e.g. Rosenthal et al. 1999; Asplund et al. 2000b,c, 2004a,c). However, it was still thought best if the most modern version of the simulations available were used, if brand new model atmospheres must be generated. For this reason, a version of the Stein-Nordlund code in use by Trampedach (2004) was employed rather than the slightly older version (Asplund et al. 2000b) used to generate the Phase 1 model. The newer code contained an improved treatment of the numerical viscosity, and drew on an updated Uppsala package containing improved continuous opacities. The version of the MHD equation of state was also more recent, including the 17 most abundant solar elements (as opposed to the previous 16, where argon was not included) as well as drawing on slightly altered abundances. The manner in which radiation pressure and energy was included by the MHD tabulation program was also altered. Finally, the mean density and temperature structures used in each case to generate equation of state and opacity tables were slightly different, though it is not clear whether this was a primary difference or a secondary effect caused by other updates.

Line formation simulations were carried out for all lines in Table B.1 on each of the four new atmospheres. Each new atmosphere had been run for 120 snapshots, though due to some relaxation effects early in the new simulations (caused by the combination of the newer code and altered extent and/or boundary condition), some earlier snapshots were not used in the final production of line profiles and bisectors. The starting snapshot of the simulations was the same as the starting snapshot of the Phase 1 model, itself taken from a previous simulation. The final snapshot of each new atmosphere also contained a computational artefact, arising from a bug in an existing snapshot manipulation utility

Figure 7.7: Differences between observed and synthetic bisectors generated with the Phase 3-82 model for all 31 lines. In comparison to Fig. 7.2, the large discrepancy in the upper parts of the bisectors has been remedied, reflecting the ‘turning-back’ of bisector tops by the improved model. The improvement over the Phase 1 bisector agreement is at least as good as that produced by the Phase 2-v16 model (Fig. 7.5), resulting in very good agreement overall between observed and theoretical bisectors.



used to implant the starting snapshot, so the final profiles and bisectors are a temporal average of a 105-snapshot period extending from snapshot 11 to snapshot 115 inclusive.

7.3.2 Results

Each new hydrodynamic simulation ran for a little over 3 days on a 1.2 GHz, 4 GB RAM, Sun-Fire-280R, followed by the 31×4 half hour radiative transfer simulations. Amazingly, *all four models* generated the correct asymmetries, reproducing the ATMOS bisectors at least as well as model v16 of Phase 2. Profiles in each case were in far better agreement than with any previous model; the average reduced χ^2 values produced by the new models were 0.087 (standard deviation 0.044), 0.121 (standard deviation 0.082), 0.344 (standard deviation 0.357) and 0.234 (standard deviation 0.204) for Phase 3-82, -82e, -88 and -88e respectively, all much lower than either the Phase 1 or Phase 2 values of around unity.⁴ Also slightly surprisingly, almost no difference could be seen with the naked eye between the profiles and bisectors produced by the four different models. For this reason, combined with the χ^2 values of the four and the fact that the original domain and boundary condition were the established configuration, the Phase 3-82 model was chosen for detailed analysis and discussion.

The same example profiles and bisectors as shown for Phase 1 and Phase 2 are displayed for the Phase 3-82 model in Fig. 7.6. Bisector differences for the entire line list are plotted in Fig. 7.7, showing significant improvement over the Phase 1 equivalent plot (Fig. 7.2), and even some improvement over the Phase 2-v16 plot (Fig. 7.5). The analysis of line shift performed for the Phase 1 model is repeated for the Phase 3-82 case in Fig. 7.8, whilst the scatter in post-fitting line depths for Phase 1 and Phase 3-82 are compared in Fig. 7.9 The average temperature structures of the two models are shown in Fig 7.10.

⁴As discussed in §7.1.4, the χ^2 values are unusually low and only useful for comparative purposes, due to the overprediction of errors in the ATMOS data and the influence of the continuum on the fit.

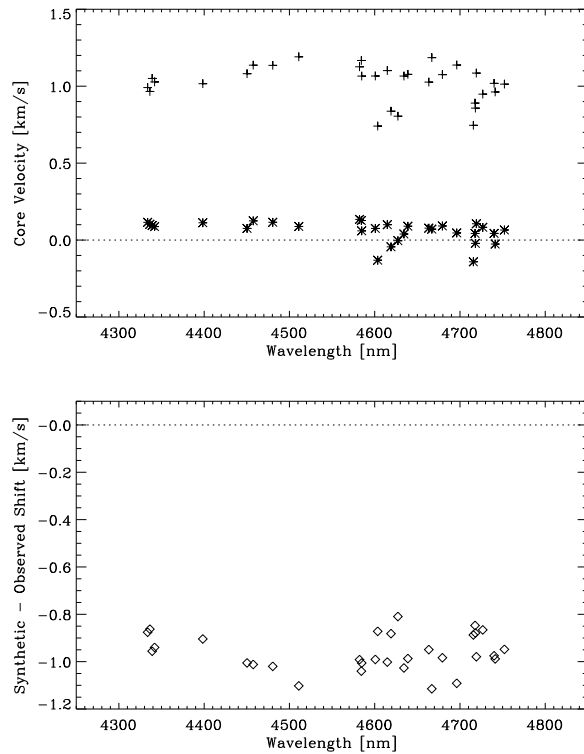


Figure 7.8: *Top:* Unfitted line core shifts in the observed (+) and Phase 3-82 modelled lines (*). Following the improvements since the Phase 1 model, observed profiles still appear very strongly redshifted, confirming the previous (Fig. 7.3) suggestion of error in laboratory or ATMOS wavelengths. *Bottom:* Difference between observed and modelled shifts. Now that the model atmosphere properly reproduces CO line profiles and bisectors (cf. Figs. 7.6 and 7.7), this plot can be confidently concluded to illustrate an approximate systematic error in laboratory wavelengths or ATMOS wavelength calibration of $0.9\text{--}1.0\text{ km s}^{-1}$.

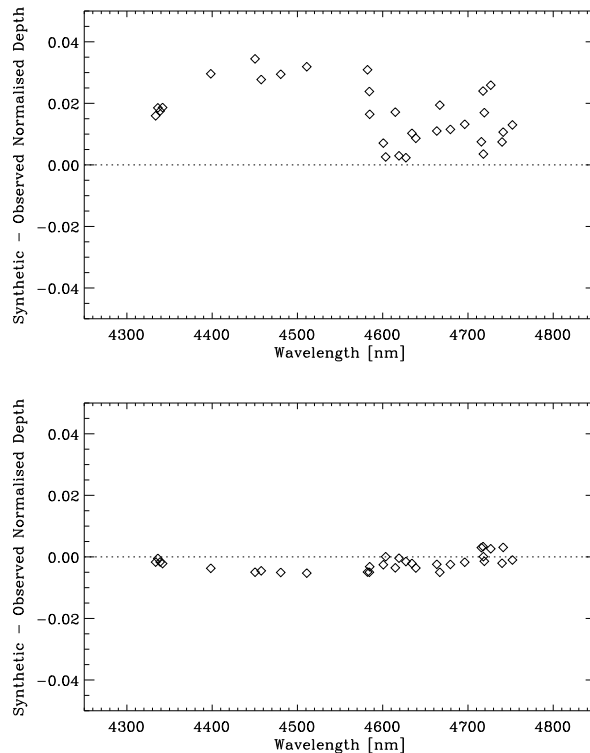


Figure 7.9: *Top:* Difference between observed and modelled profile depths produced by the Phase 1 model following fitting. Large discrepancies and a large scatter within the discrepancies are clearly evident. *Bottom:* The same, but for profiles generated using the Phase 3-82 model. A drastic reduction in discrepancy and discrepancy scatter can be seen, reflecting the greatly improved profile fits made possible by the Phase 3-82 model, thanks to its more correct overall description of line shape.

7.3.3 Discussion

Model Comparisons

The lack of any difference in result by the $z=82$ and $z=88$ models suggests that gas entering the simulation from the upper boundary does indeed have sufficient time to equilibrate with its surroundings by the time it reaches the height of strong CO line-formation. This is hence clearly not the reason for the Phase 1 model's mistaken description of the uppermost parts of the intergranular lanes. In fact, the agreement of the extended simulations with observation was possibly less good than their non-extended counterparts, as seen by the respective χ^2 values, though this can't be said with certainty given the χ^2 standard deviations. We interpret this as possibly indicative of the poor description afforded in these higher layers by LTE, ICE, the MHD equation of state and the lack of magnetic fields, such that the extended layers might even be causing some feedback upon and actually damaging the simulation below 1 Mm. The altered boundary condition performed more or less as expected, producing slightly poorer fits than the original condition in the lower simulation but improving things slightly in the higher model, though these differences are not really statistically significant given the size of standard deviations in χ^2 . If anything, the performance of the original boundary condition in the Phase 3-88 model was perhaps better than anticipated.

Despite the failure of the domain extension and its associated hypothesis, an enormous overall improvement in agreement with ATMOS bisectors and profiles was seen, with a better than order of magnitude improvement in reduced χ^2 . In a very surprising twist, the hydrodynamical simulations appear at first glance to have been sufficiently improved for the deficiencies in the upper lane areas of Phase 1 to have been removed. Conjecturalising as to exactly which minute change or combination of changes described in §7.3.1 is responsible for such a higher-order effect as the turning of one end of a bisector is exceedingly difficult. All that can confidently be said on this matter is that it is very unlikely the introduction of argon to the equation of state had any effect. Beyond this, any combination of the tiny changes in opacity and abundance inputs, viscosity and radiation pressure treatments or initial mean structure could be responsible. A systematic study of the differences could be performed and an answer arrived at, but it would be of little import, and probably rather uncertain anyway.

However, whether the improvement is attributable to resolutional effects rather than actual model differences must be considered. Asplund et al. (2000a) showed that there is an increase in strong Fe line width going from the resolution of the Phase 3 models to that of the Phase 1 model, with a preferential filling in of the bluewards wing of profiles over the redwards wing. This is due to the asymmetric way in which low resolution models truncate the vertical velocity distribution, removing more of the high upwards than downwards velocities. This correspondingly manifests itself in a bluewards turning of bisector tops with higher resolution, or equivalently, as a redwards 'turning-back' of bisectors with insufficient resolution.

This 'turning-back' has certainly occurred in the current study, so the important question is now not whether, but to what extent the improved bisectors and profiles are attributable to the lower resolution. The bisectors of Asplund et al. (2000a) show a maximum redshifting of the bisector top of 1.5 km s^{-1} with the change from a $200 \times 200 \times 82$ to $50 \times 50 \times 82$ model. They also show a redwards shifting of bisector feet of approximately 1.0 km s^{-1} . The Phase 3-82 model bisectors on the other hand demonstrate a bare minimum of 2.5 km s^{-1} shift in the bisector top from Phase 1, whilst there is vir-

tually no shift evident in bisector feet. The difference in χ^2 values between the Phase 1 and Phase 3-82 models is also far greater than could be explained purely by resolutional effects. On the basis of this difference as well as abundance-related and temperature considerations discussed in the following sections, we estimate the contribution of resolutional effects as certainly less than half of the improvement seen.

Line Depths, Shifts and Strengths

The improvement of profile shapes with the Phase 3-82 model over the Phase 1 version is borne out by an improved convergence in fitted line depths and strengths. Fig. 7.9 shows line depth agreement between synthetic and observed profiles after fitting for both the Phase 1 and Phase 3-82 model atmospheres. The drastically reduced scatter and discrepancy values of the lower graph are a striking illustration of the fact that the Phase 3-82 atmosphere allows a much closer fit with observations than its predecessor.

Similarly, the fitted abundance parameters of the 31 lines show far less scatter in the case of the Phase 3-82 model. The average implied abundance is also a lot more believable, with Phase 1 producing $\log \epsilon_C = 8.75 \pm 0.16$ and Phase 3-82 $\log \epsilon_C = 8.44 \pm 0.09$. This latter abundance is more reasonable because the value currently thought most accurate is the $\log \epsilon_C = 8.39$ recently derived by Asplund et al. (2004a). This improvement roughly indicates that equivalent widths produced by the later model are more correct, though being strong lines the actual implied abundances should not be considered very reliable. As discussed in §5.1, this is because strong lines give inconsistent abundance measures due to their dependence upon γ and correspondingly nonlinear local curves of growth. They are also more affected by any inadequacies in the model atmosphere, which will be most evident at height rather than near the surface, as plainly seen here. Proper analysis of abundance indications by CO lines is the focus of Chapter 8. The change in fitted abundances does however support the notion that resolutional effects do not play a dominant role in the bisector and profile improvements, as the effect of reduced resolution upon abundance is generally the *opposite* of that observed, i.e. an increase in average abundance and scatter (Asplund et al. 2000a).

The fitted line shifts from the Phase 3-82 run shown in Fig. 7.8 are near identical to those produced in Phase 1. However, now that excellent spectral agreement has been achieved between observation and model, they can be confidently used as a quantitative estimator of the systematic wavelength error. Hence, it appears that either the CO laboratory wavelengths or the ATMOS wavelength calibration are out by $0.9\text{--}1.0 \text{ km s}^{-1}$. Given that using the same line data and observations, Hamilton & Lester (1999) found only blueshifts in 1323 CO line cores following ‘calibration’ of their solar atlases, it seems that the ATMOS data wavelength scale is the source of this systematic error.

Inferred Temperature Structure and CO Distribution

The average temperature structures of the Phase 1 and Phase 3-82 models are very similar. The discrepancy seen in geometric height scale (the left of Fig. 7.10) reduces markedly when the two structures are considered on an optical depth scale (the right of Fig. 7.10). This reflects the slight inwards migration of the entire model atmosphere in the lower resolution case, an effect already observed by Asplund et al. (2000a). The discrepancy exists on the geometrical depth scale because the zero depth in the simulations is hard-set rather than allowed to vary with the exact position of $\langle \tau_{500} \rangle = 1$. The difference in geometric temperature structures shown in the lower right of Fig. 7.10 is similar to that

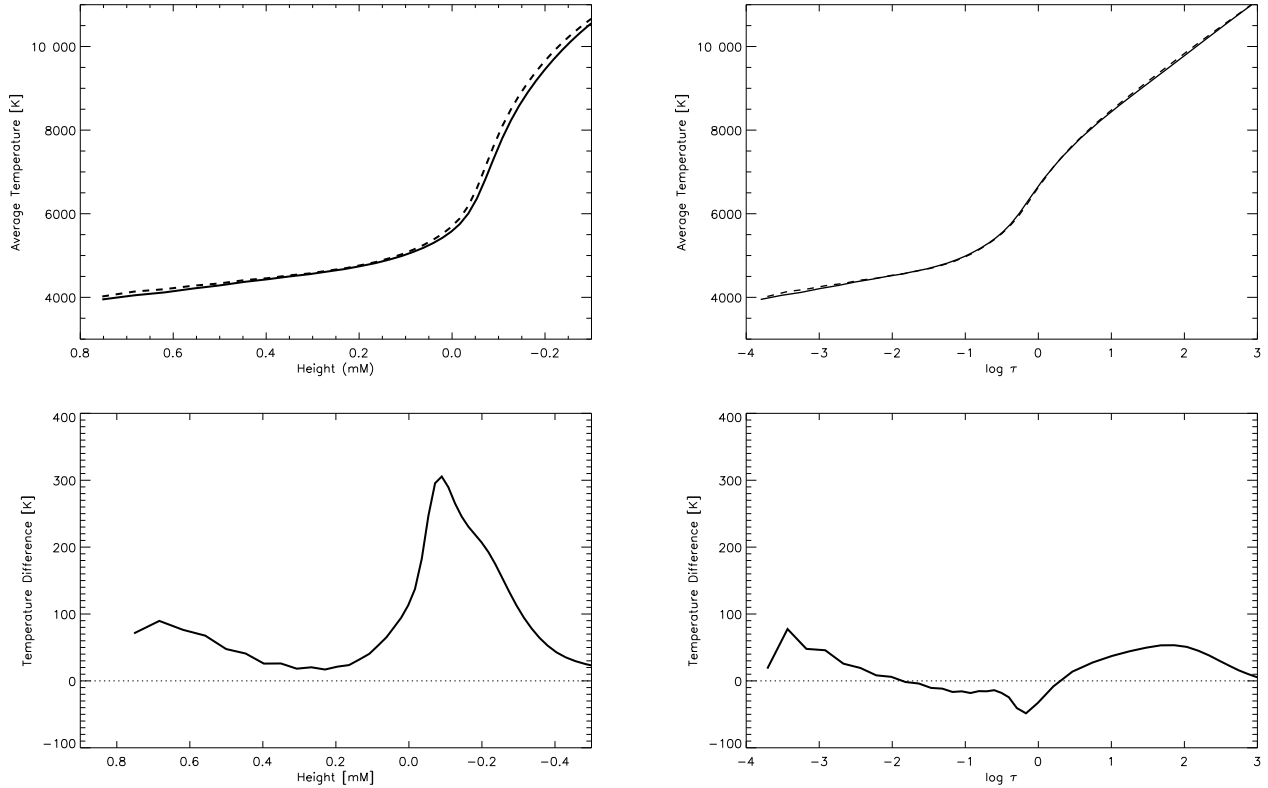


Figure 7.10: Comparison of Phase 1 (dashed line) and Phase 3-82 (solid line) model temperature structures. *Left:* Temperature structures on a geometric depth scale (top), and their difference (bottom). The entire temperature structure of the Phase 3-82 model is evidently shifted slightly inwards relative to its predecessor. *Right:* Temperature structures (top) and their difference (bottom), on a mean optical depth scale derived by averaging optical depths at respective geometrical depths. Remaining differences in temperature structure even on an optical depth scale indicate that the geometric shifting is not the only temperature effect of the new model. To what extent the reduced resolution of the Phase 3-82 model is responsible for these temperature differences is discussed in the text.

found by Asplund et al. (2000a), with the exception of the highest peak. This difference near to the solar surface is much greater than the purely resolutional effect (which is a peak about a third the height), probably reflecting the altered abundances and opacities' influence upon continuum formation. This difference underlines the point that the Phase 3 models do indeed produce atmospheres different to the Phase 1 model beyond resolutional effects, though a temperature difference this low in the atmosphere likely had no effect upon the strong lines studied here.

The small drop in temperature higher in the atmosphere is certainly associated with the redshifting of bisector tops characteristic of lower resolution simulations. As already discussed however, there is good reason to believe that this is not the only or even the dominant source of bisector and profile shape improvement between the Phase 1 and Phase 3-82 models. Regardless, the 'resolutional assistance' in turning bisector tops indicates that *both* the Phase 1 and Phase 3-82 versions of the hydrodynamical code (were the latter to be run at a full resolution) produce atmospheres with slightly ($\sim 100\text{K}$) higher mean temperatures in the highest layers than they should. Given the results of Phase 2, this is probably due to overprediction of temperatures above intergranular lanes. Hence, despite the fact that its small upper drop was achieved predominantly via resolutional effects, the Phase 3-82 temperature structure is probably a reasonably accurate description of the mean properties of the Sun. If anything, this temperature structure may possibly still be marginally too warm in the uppermost layers, as evidenced by the still slightly less curved nature of modelled bisectors than observed ones (Fig. 7.7).

Having essentially achieved the goal of proper description of CO line profile shapes and asymmetries, the Phase 3-82 model temperature structure can be brought to bear upon the COMosphere debate. The solid line temperature structure of Fig. 7.10 coupled with the now excellent CO agreement between ab initio model and observation unequivocally demonstrate the existence of cool gas in the lower chromosphere. In fact, the temperature at the site of the previous 'minimum' is also lower than previously thought, at 4200 rather than 4500K. The 3900-4100K characteristic temperature of the COMosphere though is a little warmer than the 3500K proposed by Ayres (2002). However, owing to the heterogeneity of the model utilised here, we find evidence for the presence of some persistent gas with temperatures as low as 3700K at COMospheric heights, as well as intermittent gas temperatures reaching as low as 2000K. Whilst these stated temperatures maybe could be too warm due to the possible overprediction of temperature by even the Phase 3-82 model, they are not thought to be very much overestimated, seeing as the remaining bisector discrepancy is small.

The lack of any profile or bisector improvement in the extended simulations indicates that the extra layers certainly do not contribute to CO line formation. This also suggests that the downflowing gas entering the upper layer of the non-extended simulations does not play a role in disc centre CO line formation until it has passed significantly beyond the top boundary layer and been permitted to cool to the temperature of the surrounding intergranular lanes. Hence, gas above a height of 0.75 Mm can be identified as also not contributing to solar CO line formation. As it will take some distance to achieve temperature equilibration, our results demonstrate an uppermost effective extent of the COMosphere of around 700 km, in excellent agreement with the indications of Asensio Ramos et al. (2003). It should be noted however that this does not preclude the existence of cool(er) gas at greater heights, just defines the uppermost extent of CO in *significant* concentrations.

Comparisons with Previous Work

The study described in this chapter represents a significant step forward from the only other 3D investigation of CO line formation to date (Uitenbroek 2000a). This study has utilised two modern incarnations of the Stein-Nordlund models, one the most updated version available and the other a slightly older but well proven version running at a full $200 \times 200 \times 82$ resolution. The previous study on the other hand, was based upon the very early Stein & Nordlund (1989) version, running at a resolution of $63 \times 63 \times 63$. The current study produced profiles spatially averaged over the entire simulation domain and temporally averaged over either 99 or 105 snapshots corresponding to about an hour of solar time, whereas that of Uitenbroek (2000a) used a vertical slice through a single snapshot. The maximum vertical extent of the current study was about 1.2 Mm, compared with 0.6 Mm in the earlier work. Final agreement between the modelled spectrum and observation was excellent, with analysis proceeding and agreement found down to the level of individual line bisectors. The overly deep CO line cores found by Uitenbroek appear, as suggested by Asensio Ramos et al. (2003), to have been caused by too cool a version of the 3D model atmospheres. The recently reduced solar carbon and oxygen abundances (Asplund et al. 2004a,c) have also contributed to the success of the current study, permitting the deviation of line profiles from the Grevesse & Sauval (1998) abundances in order to improve agreement with observation. This option was not realistically available to Uitenbroek (2000a) given prevailing wisdom at the time, and in light of the current results this probably also contributed to his modelled overprediction of CO line depths.

C and O Isotopic Abundance Determinations

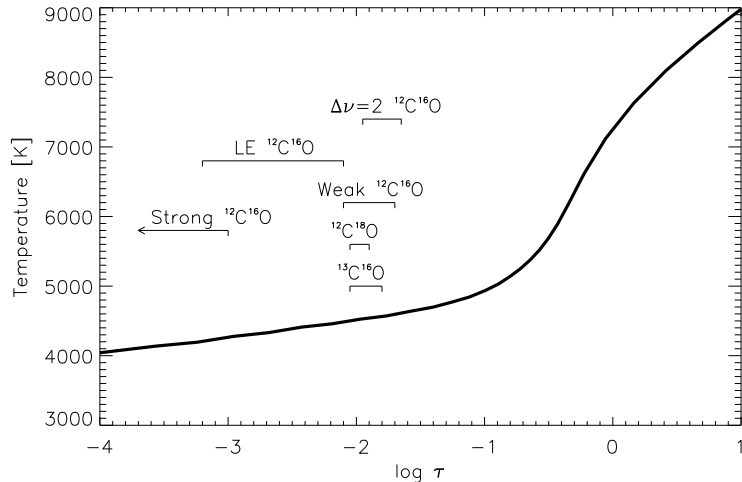
8.1 Line Lists

Five sets of CO lines were utilised in this study, once more provided by Grevesse & Sauval (2004) with gf values from Goorvitch & Chackerian (1994). Equivalent widths were also computed and provided by Grevesse & Sauval (2004). The primary investigation was performed with a set of 13 weak $^{12}\text{C}^{16}\text{O}$ lines (Table B.2), as well as sets of 16 $^{13}\text{C}^{16}\text{O}$ (Table B.3) and 15 $^{12}\text{C}^{18}\text{O}$ (Table B.4) lines. These lines all have much lower formation heights than the strong $^{12}\text{C}^{16}\text{O}$ lines considered for the previous study, as illustrated in Fig. 8.1. Being CO features, in absolute terms these lines still form reasonably high in the atmosphere, but they were selected as forming low enough for abundance determination using the 3D model. The further two line lists consist of 15 low excitation (LE) $^{12}\text{C}^{16}\text{O}$ (Table B.5) and 66 first overtone ($\Delta\nu = 2$) $^{12}\text{C}^{16}\text{O}$ (Table B.6) lines. The LE lines are formed across a broad optical depth range high in the atmosphere (due to the low temperatures required for significant populations in the lower energy levels), and the $\Delta\nu = 2$ at around the same height as the three primary sets (Fig. 8.1). These supplementary lists were used to derive alternative carbon abundances (and hence isotopic ratios) to the primary $^{12}\text{C}^{16}\text{O}$ list, exploring the abundance performance of the model over higher layers and overtone bands. The three different $^{12}\text{C}^{16}\text{O}$ line lists have traditionally produced widely varying carbon abundance measures using 1D models (Grevesse & Sauval 2004), so a consistent result in 3D would greatly increase confidence in the new C abundance and isotopic ratios. Again, all lines were also selected to be free of blending.

8.2 Dealing with CO and Isotopes

Because oxygen is far more abundant than carbon in the solar photosphere, CO concentration is most sensitive to carbon rather than oxygen abundance. For this reason, a fitted difference from input abundance for CO lines can be approximately interpreted as a difference in solar carbon abundance, even though strictly speaking it is actually indicative of a difference in CO abundance at the height of line formation. Therefore, in order to use CO lines to derive a solar carbon abundance, the input carbon abundance was iteratively altered according to the average fitted abundances of the CO lines from the previous iteration, until only small abundance changes remained. The oxygen abundance does shift the equilibrium position of the CO formation-dissociation reaction somewhat, and even though this influence is not as significant as that of carbon, carbon abundances derived in

Figure 8.1: Approximate optical depths of core formation for the different CO line populations used in this chapter (all but strong $^{12}\text{C}^{16}\text{O}$) and the previous (strong $^{12}\text{C}^{16}\text{O}$ only). The temperature structure shown is that of the standard (Asplund et al. 2000b) model atmosphere used both in this chapter and Phase 1 of the previous chapter.



this manner are therefore dependent upon oxygen abundance. Input oxygen abundances were therefore carefully chosen (see §8.3) and kept constant throughout the study.

Using the above technique, the solar ^{12}C abundance was determined separately using the three different $^{12}\text{C}^{16}\text{O}$ line lists. Since the 3D model input abundances do not differentiate between isotopes, these determinations were performed by altering the total input carbon abundance, though the final abundance arrived at is not overall abundance, but the carbon abundance *if all C in CO were contained in $^{12}\text{C}^{16}\text{O}$* . This can approximately be called the ^{12}C abundance, even though it does not include any ^{12}C tied up in $^{12}\text{C}^{17}\text{O}$ or $^{12}\text{C}^{18}\text{O}$, though their contribution will be minimal given the high values of $^{16}\text{O}/^{18}\text{O}$ and $^{16}\text{O}/^{17}\text{O}$.

The concentrations of $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ relative to $^{12}\text{C}^{16}\text{O}$ are identical to the $^{12}\text{C}/^{13}\text{C}$ and $^{16}\text{O}/^{18}\text{O}$ ratios. In order to determine the concentrations of the CO isotopomers, given the lack of provision for isotopic differentiation in the model, the isotopic lines were treated in the radiative transfer simulations as if they were created by $^{12}\text{C}^{16}\text{O}$. In order to do this correctly, the radiative transfer code had to be altered (`rayt` and `trline` in §A.2) to include provision for a **mass scalefactor** and an **opacity scalefactor**. The mass scalefactor allowed the correct molecular mass to be used in the line formation calculations, and was simply the ratio of the mass of the isotopomer in question to that of the most common isotopomer (i.e. $^{12}\text{C}^{16}\text{O}$). These factors, 1.03583 for $^{13}\text{C}^{16}\text{O}$ and 1.07157 for $^{12}\text{C}^{18}\text{O}$, were calculated from nuclear weights given by Audi & Wapstra (1995).

The opacity scalefactor contained the information about different isotopomer concentrations and therefore the atomic isotopic ratios, as the line opacities for any particular transition in two different isotopomers are proportional to their densities. The use of an opacity scalefactor was preferable to simply altering the input carbon abundance in order to emulate the difference in isotopic abundances. This is because the overall carbon abundance was not altered and therefore did not feed back on other parts of the simulation like CN line formation or the temperature structure, which might in turn indirectly effect CO line formation. The opacity scalefactor was necessary anyway, in order to include an actual molecular difference (rather than just that due to abundances) in opacity between isotopomers. This opacity correction arises as follows (after the suggestions of Grevesse & Sauval 2004).

Consider two isotopomers of a diatomic molecule of elements X and Y: ‘ $\mathcal{A}$ ’ = $^a\text{X}^c\text{Y}$

and ‘ $\mathcal{B}$ ’ = ${}^b\text{X}^c\text{Y}$. Now, the opacity of a species in a given transition depends on the density of absorbers, the transition probability and the relevant line broadening effects. In the case of a weak lines, as those considered in this study are, Doppler broadening given by the profile ϕ_D from Eq. 2.9 can be approximated as the only significant contributor to the latter, meaning that for our molecule $\mathcal{B}$,

$$\kappa_{\mathcal{B}^*} \propto N(\mathcal{B}^*) f_{\mathcal{B}^*} \phi_D \quad (8.1)$$

where $\mathcal{B}^*$ denotes the isotopomer $\mathcal{B}$ in some given energy level from which the transition in question occurs, $N(\mathcal{B}^*)$ refers to the number density of isotopomers $\mathcal{B}$ in the starred (excited) energy level and $f_{\mathcal{B}^*}$ refers to the oscillator strength or probability of the particular transition from the excited energy level. Now, at any given wavelength $\Delta\lambda$ in Eq. 2.9, we see that

$$\begin{aligned} \phi_D &\propto \frac{1}{\Delta\lambda_D} \propto \frac{1}{\sqrt{\frac{2kT}{m} + \xi_t^2}}, \\ \therefore \kappa_{\mathcal{B}^*} &\propto \frac{N(\mathcal{B}^*) f_{\mathcal{B}^*}}{\sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}}. \end{aligned} \quad (8.2)$$

Now, assuming LTE, we know from statistical mechanics (Mihalas 1978) that a Boltzmann distribution of energy levels implies that where many instances of some microscopic system Υ occur, the population of a particular excited energy level Υ^* is given by

$$N(\Upsilon^*) = \frac{N(\Upsilon) g_{\Upsilon^*} \exp(\frac{-E_{\Upsilon^*}}{kT})}{Z(\Upsilon)}, \quad (8.3)$$

where g_{Υ^*} is the statistical weight of the excited energy level, E_{Υ^*} is its energy and $Z(\Upsilon)$ is the partition function of the system. Hence,

$$\kappa_{\mathcal{B}^*} \propto \frac{N(\mathcal{B}) g_{\mathcal{B}^*} \exp(\frac{-E_{\mathcal{B}^*}}{kT}) f_{\mathcal{B}^*}}{Z(\mathcal{B}) \sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}}. \quad (8.4)$$

Now, the number of molecules is related to the number density of the molecule’s constituent atoms, so

$$N(\mathcal{B}) = \frac{N({}^b\text{X}) N({}^c\text{Y})}{\kappa(\mathcal{B})}, \quad (8.5)$$

where $\kappa(\mathcal{B})$ is the **rate constant** of the formation-dissociation reaction of the isotopomer $\mathcal{B}$, given (Grevesse & Sauval 2004) by

$$\kappa(\mathcal{B}) \propto \frac{Z({}^b\text{X}) Z({}^c\text{Y}) \mu_{\mathcal{B}}^{\frac{3}{2}} \exp(\frac{-D_{\mathcal{B}}}{kT})}{Z(\mathcal{B})} \quad (8.6)$$

where $D_{\mathcal{B}}$ and $\mu_{\mathcal{B}}$ are the dissociation energy and reduced mass respectively of isotopomer $\mathcal{B}$. Hence, combining Eqs. 8.4-8.6 we now see that

$$\kappa_{\mathcal{B}^*} \propto \frac{N({}^b\text{X}) N({}^c\text{Y}) g f_{\mathcal{B}^*} \exp(\frac{-E_{\mathcal{B}^*}}{kT})}{\kappa(\mathcal{B}) Z(\mathcal{B}) \sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}}$$

$$\begin{aligned} & \propto \frac{N(^b\text{X})N(^c\text{Y})Z(\mathcal{B})}{Z(\mathcal{B})Z(^b\text{X})Z(^c\text{Y})\mu_{\mathcal{B}}^{\frac{3}{2}}\exp(\frac{-D_{\mathcal{B}}}{kT})} \frac{gf_{\mathcal{B}^*}\exp(\frac{-E_{\mathcal{B}^*}}{kT})}{\sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}} \\ \therefore \quad \kappa_{\mathcal{B}^*} & \propto \frac{N(^b\text{X})N(^c\text{Y})gf_{\mathcal{B}^*}\exp(\frac{(D_{\mathcal{B}}-E_{\mathcal{B}^*})}{kT})}{Z(^b\text{X})Z(^c\text{Y})\mu_{\mathcal{B}}^{\frac{3}{2}}\sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}} \end{aligned} \quad (8.7)$$

where $gf_{\mathcal{B}^*}$ and $f_{\mathcal{B}^*}$ have been combined into $gf_{\mathcal{B}^*}$, the gf value of the line.

So, the opacity scalefactor ς_{κ} for an isotopomer $\mathcal{B}$, where the reference isotopomer is $\mathcal{A}$ is then

$$\begin{aligned} \varsigma_{\kappa} & \equiv \frac{\kappa_{\mathcal{B}^*}}{\kappa_{\mathcal{A}^*}} = \frac{\frac{N(^b\text{X})N(^c\text{Y})gf_{\mathcal{B}^*}\exp(\frac{(D_{\mathcal{B}}-E_{\mathcal{B}^*})}{kT})}{Z(^b\text{X})Z(^c\text{Y})\mu_{\mathcal{B}}^{\frac{3}{2}}\sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}}}{\frac{N(^a\text{X})N(^c\text{Y})gf_{\mathcal{A}^*}\exp(\frac{(D_{\mathcal{A}}-E_{\mathcal{A}^*})}{kT})}{Z(^a\text{X})Z(^c\text{Y})\mu_{\mathcal{A}}^{\frac{3}{2}}\sqrt{\frac{2kT}{m_{\mathcal{A}}} + \xi_t^2}}} \\ & = \frac{N(^b\text{X})gf_{\mathcal{B}^*}Z(^a\text{X})\mu_{\mathcal{A}}^{\frac{3}{2}}\exp(\frac{(D_{\mathcal{B}}-E_{\mathcal{B}^*})}{kT})\sqrt{\frac{2kT}{m_{\mathcal{A}}} + \xi_t^2}}{N(^a\text{X})gf_{\mathcal{A}^*}Z(^b\text{X})\mu_{\mathcal{B}}^{\frac{3}{2}}\exp(\frac{(D_{\mathcal{A}}-E_{\mathcal{A}^*})}{kT})\sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}}, \end{aligned} \quad (8.8)$$

Now, we make the approximations $gf_{\mathcal{B}^*} \approx gf_{\mathcal{A}^*}$, $D_{\mathcal{B}} \approx D_{\mathcal{A}}$ and $E_{\mathcal{B}^*} \approx E_{\mathcal{A}^*}$, since $\mathcal{A}$ and $\mathcal{B}$ are very nearly the same molecule so their transitions and energy levels will be almost identical. Further, assuming $Z(^b\text{X}) \approx Z(^a\text{X})$ due to the first-order dependence of atomic orbitals upon charge (and not mass), we arrive at

$$\varsigma_{\kappa} = \frac{N(^b\text{X})\mu_{\mathcal{A}}^{\frac{3}{2}}\sqrt{\frac{2kT}{m_{\mathcal{A}}} + \xi_t^2}}{N(^a\text{X})\mu_{\mathcal{B}}^{\frac{3}{2}}\sqrt{\frac{2kT}{m_{\mathcal{B}}} + \xi_t^2}}. \quad (8.9)$$

where the final scalefactor is independent of transition. The reduced mass opacity corrections used for $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ were therefore 0.9346 and 0.9293 respectively, where nuclear masses were again sourced from Audi & Wapstra (1995). In practice, the ratio of the square root terms enters the opacity anyway through the mass scalefactor, and the microturbulent velocity is not used in 3D (i.e. $\xi_t = 0$ was used) so these can be disregarded also. The total opacity scalefactor applied in each case was therefore the product of the appropriate one of the reduced mass correction factors and the ratio of reference (^{12}C or ^{16}O) isotope to that involved in the line being modelled (^{13}C or ^{18}O), i.e.

$$\varsigma_{\kappa} = \frac{N(^b\text{X})}{N(^a\text{X})} \left(\frac{\mu_{\mathcal{A}}}{\mu_{\mathcal{B}}} \right)^{\frac{3}{2}} \equiv \left(\frac{^b\text{X}}{^a\text{X}} \right) \left(\frac{\mu_{\mathcal{A}}}{\mu_{\mathcal{B}}} \right)^{\frac{3}{2}} \quad (8.10)$$

The opacity scalefactors were then iteratively altered in calculations of the $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ line lists to reflect different isotopic ratios, in the same manner as the bulk carbon abundance was iterated to determine the ^{12}C abundance using the three sets of $^{12}\text{C}^{16}\text{O}$ lines. The same bulk carbon abundance as used in the final iteration of the weak $^{12}\text{C}^{16}\text{C}$ calculation was used in each case, and the isotopic ratios after some iteration i given by

$$\left(\frac{^b\text{X}}{^a\text{X}} \right)_i = \left(\frac{^b\text{X}}{^a\text{X}} \right)_{i-1} \frac{10^{\Delta^{12}\text{C}_{final}}}{10^{\Delta^{12}\text{C}_{iso_i}}}. \quad (8.11)$$

Here Δ_{iso_i} and $\Delta^{12}\text{C}_{final}$ are the abundance corrections produced by the i th isotopomer iteration and the final iteration of whichever $^{12}\text{C}^{16}\text{O}$ list is used to indicate the ^{12}C abundance, respectively.

A further iteration was performed on each of the sets of $^{12}\text{C}^{16}\text{O}$ lines, where a **fractional scalefactor** was introduced, accounting for the fact that not all carbon in CO lines exists in $^{12}\text{C}^{16}\text{O}$. This scalefactor was calculated from the just derived $^{12}\text{C}/^{13}\text{C}$ and $^{16}\text{O}/^{18}\text{O}$ ratios, such that

$$\begin{aligned}\zeta_{frac} &= \frac{N(^{12}\text{C}^{16}\text{O})}{N(\text{CO})} \\ &= \frac{N(^{12}\text{C}^{16}\text{O})}{N(^{12}\text{C}^{16}\text{O}) + N(^{13}\text{C}^{16}\text{O}) + N(^{12}\text{C}^{18}\text{O}) + N(^{12}\text{C}^{17}\text{O})} \\ &= \left(1 + \frac{N(^{13}\text{C}^{16}\text{O})}{N(^{12}\text{C}^{16}\text{O})} + \frac{N(^{12}\text{C}^{18}\text{O})}{N(^{12}\text{C}^{16}\text{O})} + \frac{N(^{12}\text{C}^{17}\text{O})}{N(^{12}\text{C}^{16}\text{O})} \right)^{-1} \\ &= (1 + ^{13}\text{C}/^{12}\text{C} + ^{18}\text{O}/^{16}\text{O} + ^{17}\text{O}/^{16}\text{O})^{-1},\end{aligned}\tag{8.12}$$

Therefore, ζ_{frac} represents the fraction of the bulk carbon abundance actually indicated by $^{12}\text{C}^{16}\text{O}$ lines. Seeing as the $^{12}\text{C}^{17}\text{O}$ lines are so weak in the ATMOS spectrum, accurate derivation of the $^{16}\text{O}/^{17}\text{O}$ ratio would not have been possible in this study, so the value of $^{16}\text{O}/^{17}\text{O}$ used in the calculation of fractional scalefactors was the terrestrial value of 2630 (Rosman & Taylor 1998). Being so incredibly small, the contribution of any difference in the ^{17}O abundance between Earth and the Sun would have had almost no effect upon the resultant scalefactor. Using these fractional scalefactors, the final iterations of the $^{12}\text{C}^{16}\text{O}$ line lists indicated bulk solar carbon abundances.

8.3 Abundance Calculations

Abundance calculations for each line within a given iteration were performed in the manner described in Chapter 5. That is, three profiles with $\log gf$ values differing by 0.2 dex were calculated for each line and linearly interpolated between to arrive at the indicated abundance. The model used was that of Asplund et al. (2000b), the same model atmosphere used for all previous 3D abundance determinations described in §3.4 and the Phase 1 model of Chapter 7. This model was used for consistency and comparability with the previous abundance determinations, as well as because the Phase 3-82 model of Chapter 7 might be inappropriate given its low resolution.

Both profile and equivalent width fitting were tested upon the first iteration of the weak $^{12}\text{C}^{16}\text{O}$ lines, with virtually no difference found in calculated abundance. However, some of the lines could not be effectively profile fitted by minimising the χ^2 statistic without some form of masking, due to the presence of other nearby lines in the ATMOS spectrum. For this reason, equivalent width fitting was used for all subsequent abundance measures, as this problem was only likely to worsen when the weaker isotopic lines were considered. The same Beer-Norton apodization as used in the study of Chapter 7 (medium BNA, characteristic velocity 1.5 km s^{-1}) was also applied to each line, though more for the sake of consistency than anything else. Having been normalised to unit area as the medium Beer-Norton ILS was, convolution with any function should be an area-preserving operation, thereby not effecting line equivalent widths nor therefore the abundances determined with them. However, the influence of side lobes in a convolving ILS means that some very small

interchange between different areas in the convolved spectrum can occur, such that the line in question changes ever so slightly in area whereas the integral over the entire convolved domain remains the same. In practice, some tiny variation in measured abundance was seen following apodization, though it is not clear whether this was the effect described or simply the result of finite numerical resolution in the spectrum, convolving function and abundance interpolation. Regardless, the influence was so small as to be inconsequential. For completeness however, it should be noted that in the case of the $\Delta\nu = 2$ lines, a BNA characteristic velocity of 0.75 kms^{-1} was used, reflecting the higher resolving power of the ATMOS instrument at the shorter wavelengths of these lines (see Table B.6).

For comparative purposes, abundance calculations were carried out for all five line lists using four different models: The 3D hydrodynamic model, HM, MARCS and a contraction of the 3D model into the vertical dimension only, which will be designated 1DAV¹. The horizontal averaging used to produce the 1DAV model was performed over surfaces of common optical depth rather than geometrical height, as the optical depth scale has most relevance to line formation. All three 1D models included microturbulence of 1 kms^{-1} . Microturbulence was not fitted for in the 1D models, as they were used simply for comparative purposes rather than highly accurate determinations. The oxygen and nitrogen abundances used for the first three were the most recent values produced by Asplund et al. (2004c) with the respective models, and the nitrogen abundance for the 1DAV model was simply approximated as the 3D value in the absence of any appropriate line calculations². The oxygen abundance used for the 1DAV model was derived from the same vibration-rotation and pure vibrational OH lines as had been employed previously (Asplund et al. 2004c). Oxygen and nitrogen abundances used in the line calculations with the different models are shown in Table 8.1.

Model	3D	HM	MARCS	1DAV
$\log \epsilon_{\text{O}}$	8.66	8.85	8.80	8.70
$\log \epsilon_{\text{N}}$	7.80	7.95	7.90	7.80

Table 8.1: Oxygen and nitrogen abundances used in line formation calculations for each model in this study. 3D, HM and MARCS values are from Asplund et al. (2004c), 1DAV oxygen from Asplund (2004) and 1DAV nitrogen abundance simply set to the 3D value.

8.4 Results

Derived abundances are plotted by equivalent width, excitation potential and wavelength for each line in the weak $^{12}\text{C}^{16}\text{O}$ (Fig. 8.2), $^{13}\text{C}^{16}\text{O}$ (Fig. 8.5), $^{12}\text{C}^{18}\text{O}$ (Fig. 8.6), LE $^{12}\text{C}^{16}\text{O}$ (Fig. 8.3) and $\Delta\nu = 2$ $^{12}\text{C}^{16}\text{O}$ sets (Fig. 8.4). The only appreciable trend evident in the 3D results is with equivalent width in the case of the LE lines, though these lines do also produce a smaller trend in excitation potential in 3D. The HM and MARCS models display trends in equivalent width and excitation potential for the $^{12}\text{C}^{18}\text{O}$ lines, and excitation potential in the $\Delta\nu = 2$ lists. In addition, the MARCS model exhibits a trend with equivalent width in its LE results. In the case of the 1DAV model, no significant trends are seen except for a small slope with equivalent width in the $^{12}\text{C}^{18}\text{O}$ list.

¹‘One Dimensional AVerage’

²Nitrogen should have very little effect on CO line formation anyway.

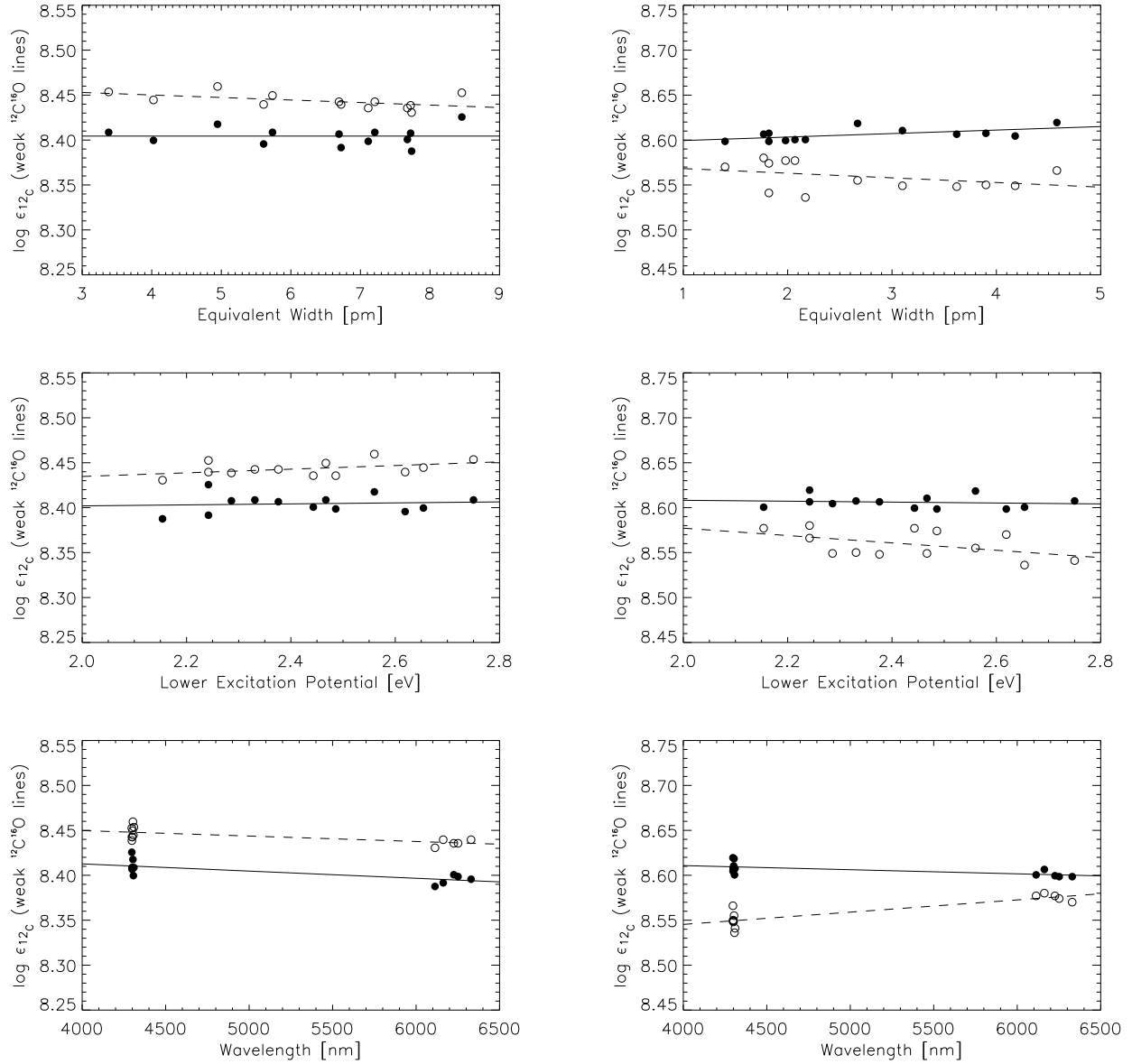


Figure 8.2: Solar carbon abundances indicated by the weak $^{12}\text{C}^{16}\text{O}$ lines, displayed according to equivalent width (top), excitation potential (middle) and wavelength (bottom). On the left, filled circles indicate 3D results and open circles 1DAV results, whilst on the right filled circles are HM values and open circles MARCS results. Trendlines are produced as linear fits to data sets using a minimised χ^2 method placing equal weight on each point, with solid lines corresponding to filled circles and dashed lines to open circles. No significant trends can be seen in the output of any model.

Model	3D	HM	MARCS	1DAV	Terrestrial
$\log \epsilon_{12\text{C}}$	8.40 ± 0.01	8.61 ± 0.01	8.56 ± 0.02	8.44 ± 0.01	
$\log \epsilon_{\text{C}}$	8.41 ± 0.02	8.62 ± 0.02	8.57 ± 0.02	8.45 ± 0.02	
$^{12}\text{C}/^{13}\text{C}$	$95.4^{+5.7}_{-5.4}$	$67.9^{+3.1}_{-3.0}$	$69.8^{+4.3}_{-4.1}$	$73.3^{+3.4}_{-3.2}$	$92.5^{+7.6}_{-6.5}$
$^{16}\text{O}/^{18}\text{O}$	532^{+43}_{-40}	344^{+30}_{-28}	350^{+35}_{-32}	376^{+31}_{-29}	487^{+36}_{-31}

Table 8.2: Abundances and isotopic ratios implied by the weak $^{12}\text{C}^{16}\text{O}$ line list as indicator of ^{12}C abundance. Note the large differences between 1D and 3D isotopic ratios. Note also that the traditional 1D models (HM and MARCS) indicate higher abundances than the 1DAV, which in turn produces a higher abundance than the 3D model.

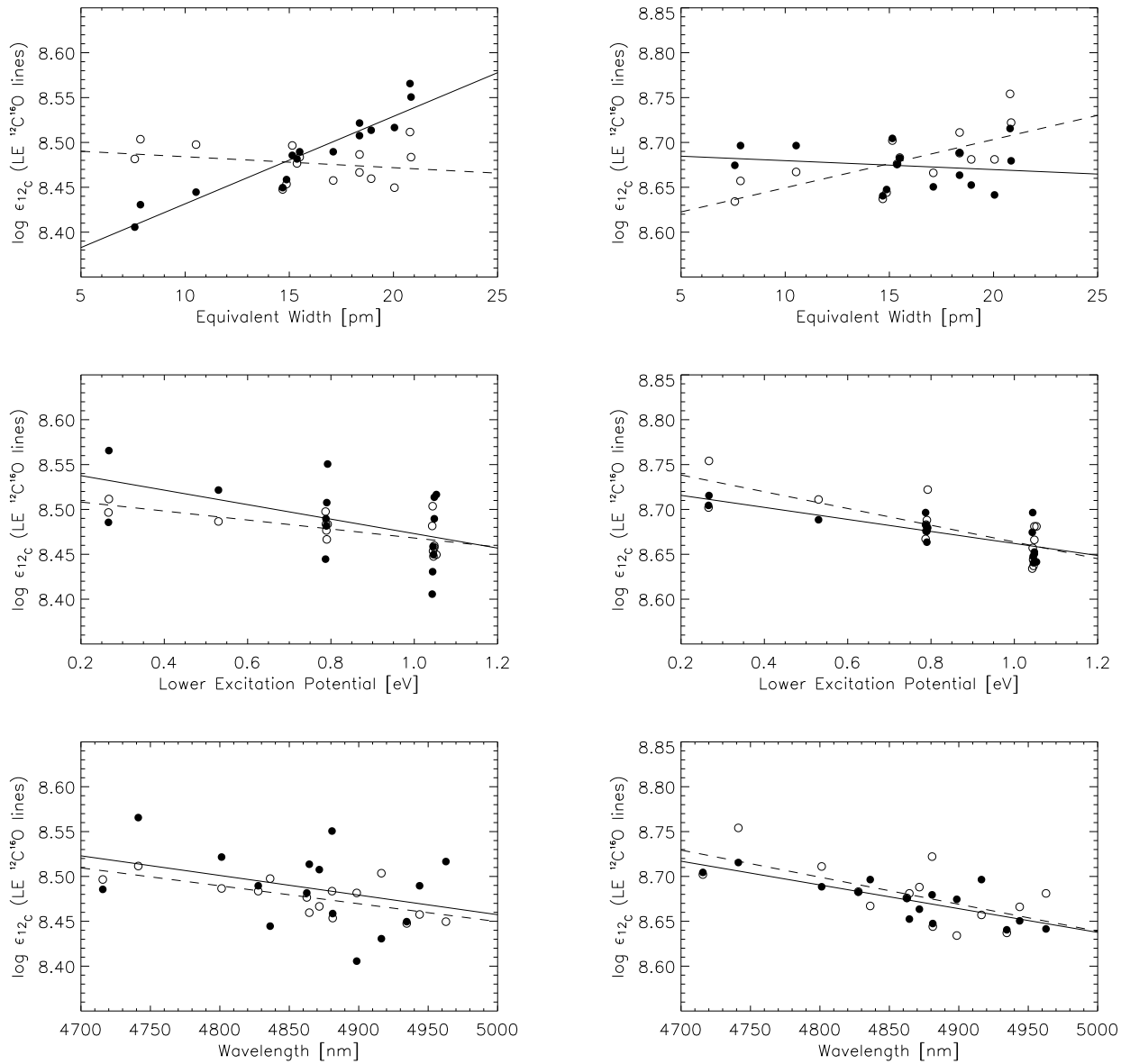


Figure 8.3: The same as Fig. 8.2, but using the LE $^{12}\text{C}^{16}\text{O}$ lines. Definite trends can be seen with equivalent width in the output of the 3D and MARCS models. Significantly, the ^{12}C abundances implied by the weakest (i.e. lowest formation height) lines in 3D are consistent with the abundances derived using the weak and $\Delta\nu = 2$ $^{12}\text{C}^{16}\text{O}$ lines. The agreement deteriorates with increased LE $^{12}\text{C}^{16}\text{O}$ line strength and therefore formation height. Less prominent trends are also evident in excitation potential for all models except 1DAV.

Model	3D	HM	MARCS	1DAV	Terrestrial
$\log \epsilon_{12\text{C}}$	8.49 ± 0.04	8.67 ± 0.02	8.68 ± 0.03	8.50 ± 0.02	
$\log \epsilon_{\text{C}}$	8.49 ± 0.05	8.68 ± 0.03	8.69 ± 0.04	8.51 ± 0.03	
$^{12}\text{C}/^{13}\text{C}$	$115.5^{+14.0}_{-12.5}$	$79.4^{+5.7}_{-5.3}$	$92.2^{+7.9}_{-8.6}$	$79.2^{+5.1}_{-4.8}$	$92.5^{+7.6}_{-6.5}$
$^{16}\text{O}/^{18}\text{O}$	644^{+86}_{-76}	403^{+42}_{-38}	463^{+57}_{-50}	407^{+39}_{-35}	487^{+36}_{-31}

Table 8.3: As per Table 8.2, but using the LE $^{12}\text{C}^{16}\text{O}$ line list as indicator of ^{12}C abundance. The same differences between models are observed as in Table 8.2.

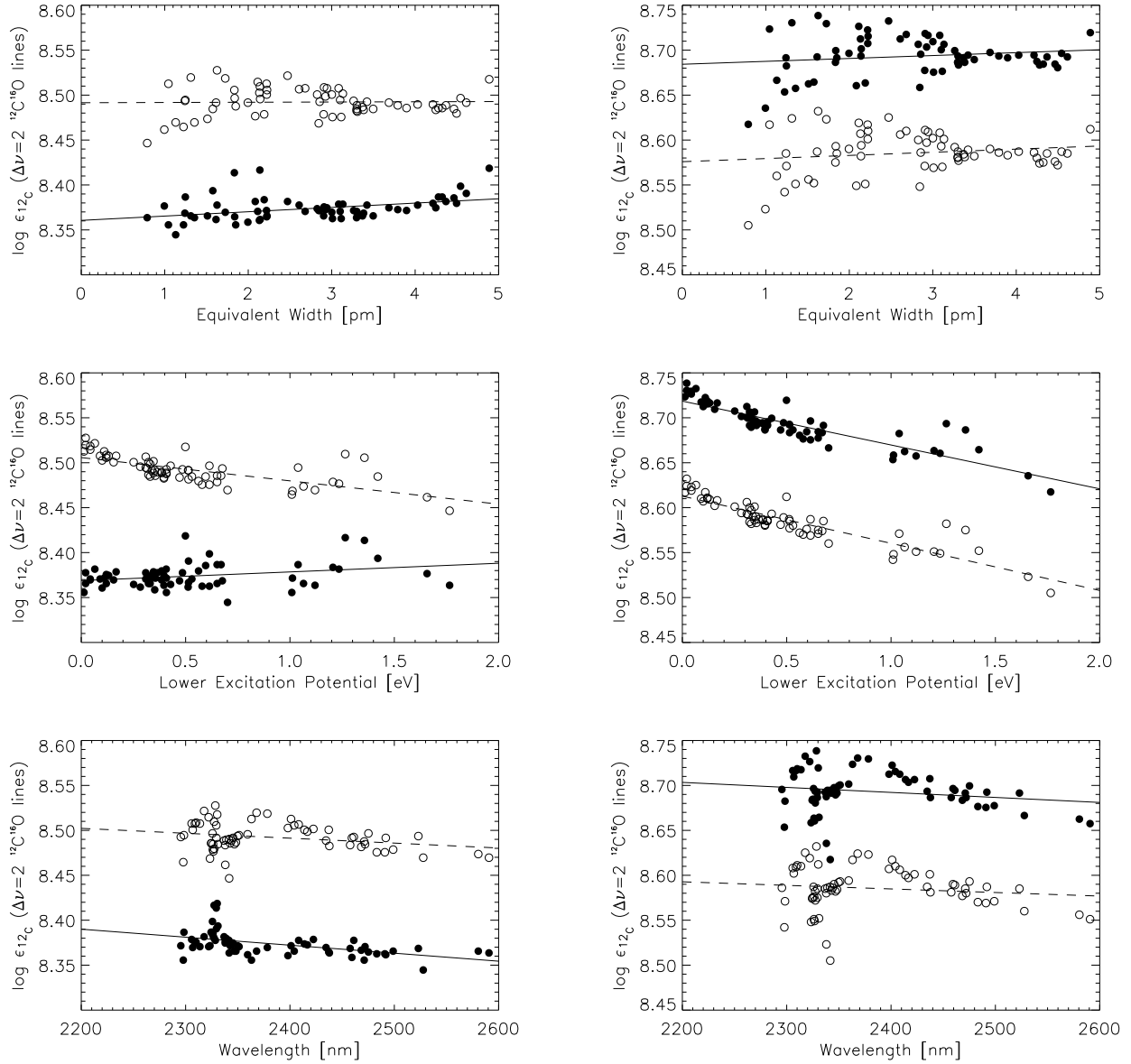


Figure 8.4: The same as Fig. 8.2, but using the $\Delta\nu = 2$ $^{12}\text{C}^{16}\text{O}$ lines. Significant trends can be seen with excitation potential in the 1D results, though none in the case of the 3D model.

Model	3D	HM	MARCS	1DAV	Terrestrial
$\log \epsilon_{12\text{C}}$	8.37 ± 0.01	8.69 ± 0.02	8.59 ± 0.02	8.52 ± 0.02	
$\log \epsilon_{\text{C}}$	8.38 ± 0.02	8.70 ± 0.03	8.59 ± 0.03	8.52 ± 0.02	
$^{12}\text{C}/^{13}\text{C}$	$89.0^{+5.6}_{-5.3}$	$83.0^{+5.8}_{-5.4}$	$74.2^{+5.6}_{-5.2}$	$82.0^{+4.6}_{-4.3}$	$92.5^{+7.6}_{-6.5}$
$^{16}\text{O}/^{18}\text{O}$	496^{+42}_{-38}	421^{+43}_{-39}	372^{+41}_{-37}	421^{+38}_{-35}	487^{+36}_{-31}

Table 8.4: As per Table 8.2, but using the $\Delta\nu = 2$ $^{12}\text{C}^{16}\text{O}$ line list as indicator of ^{12}C abundance. The same differences between models are observed as in Table 8.2.

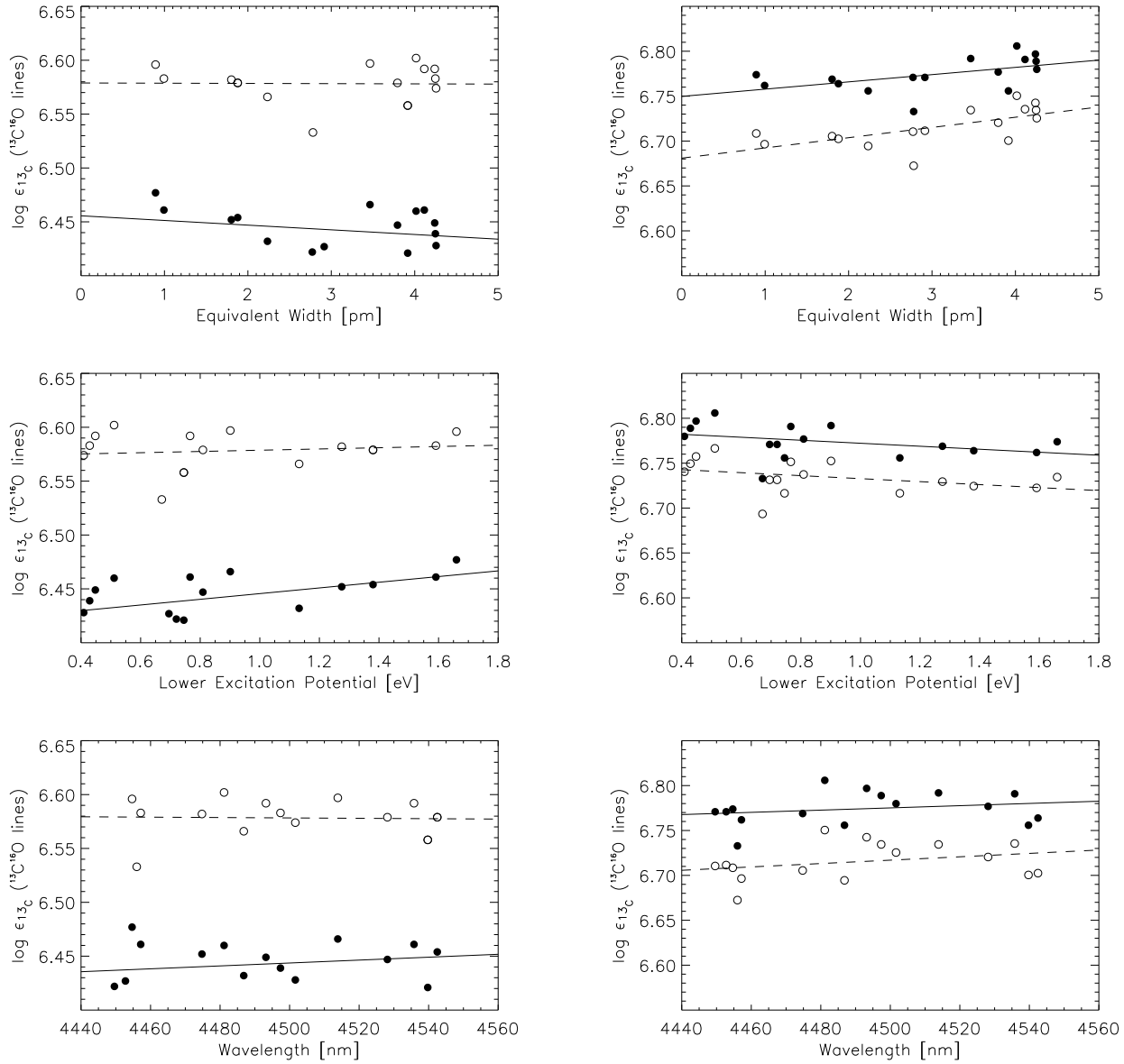


Figure 8.5: The same as Fig. 8.2, but indicating ^{13}C through the use of the $^{13}\text{C}^{16}\text{O}$ lines. No significant trends can be seen in the output of any model.

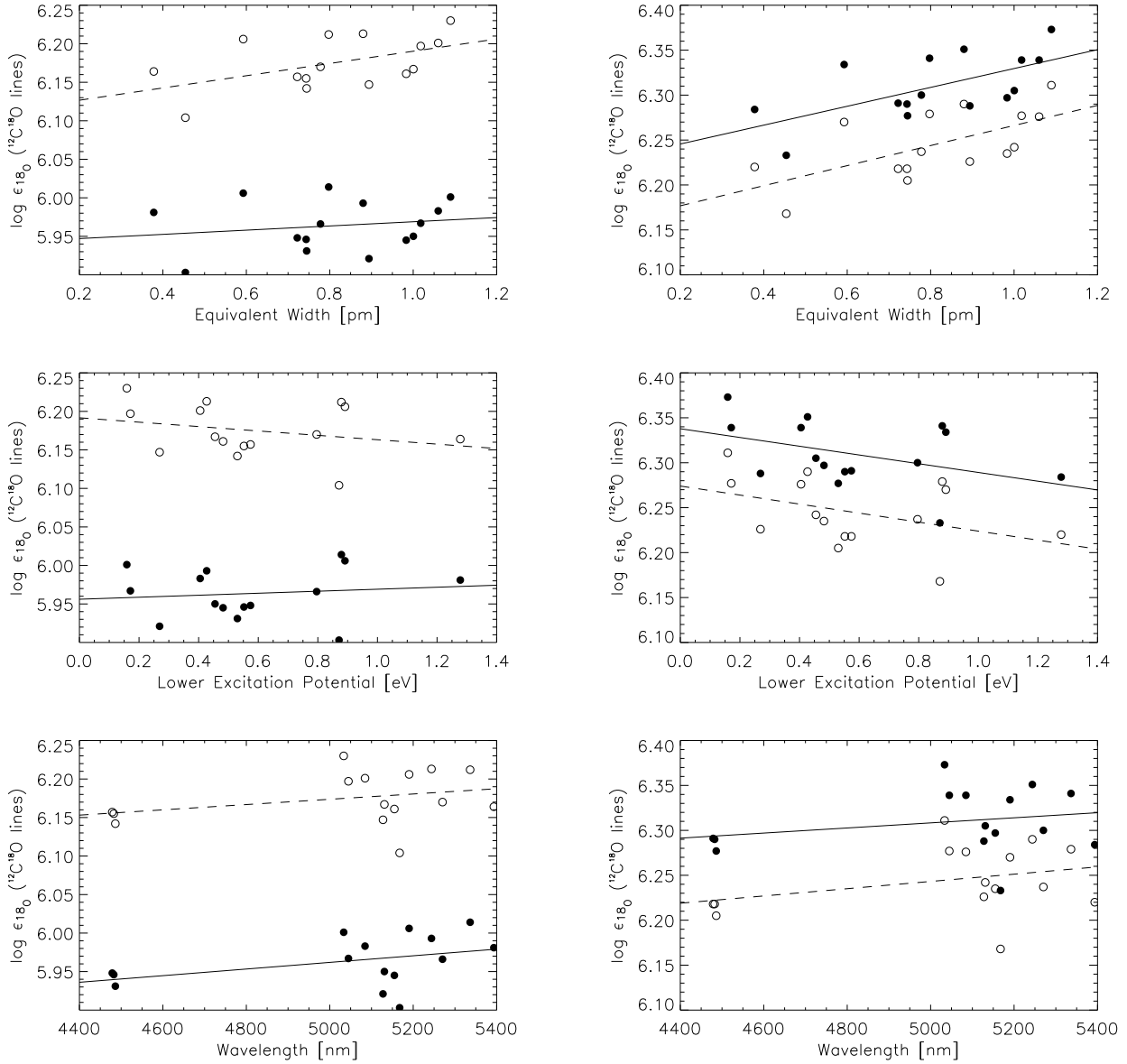


Figure 8.6: The same as Fig. 8.2, but indicating ^{18}O through the use of the $^{12}\text{C}^{18}\text{O}$ lines. Significant trends can be seen in equivalent width and excitation potential in the HM and MARCS results.

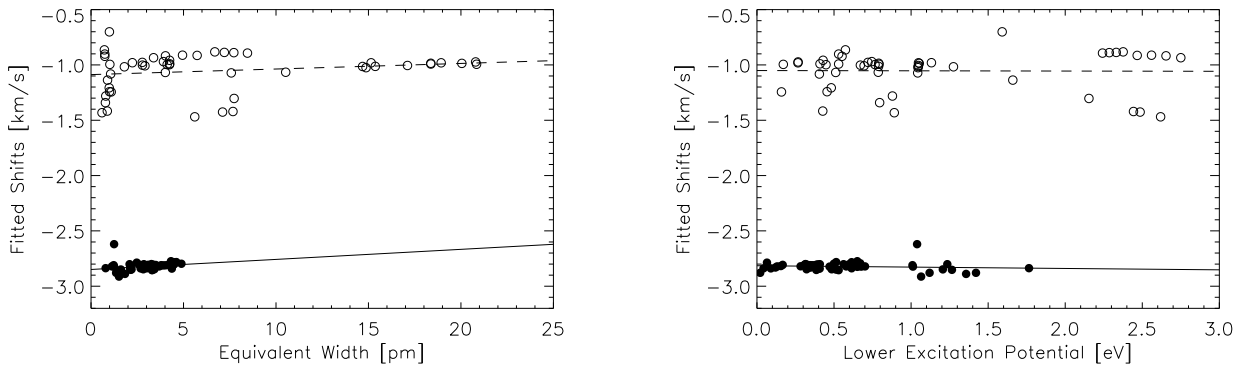


Figure 8.7: Fitted shifts for all lines sets used in this chapter. Open circles are weak, LE and isotopic lines. Here the absence of trends clearly shows a systematic error of approximately 1.0 km s^{-1} in reference wavelengths, consistent with the findings of §7.3.3. Filled circles are $\Delta\nu = 2$ lines, with the absence of significant trends showing that the ATMOS wavelength calibration error implied by the other lines translates to about a 2.8 km s^{-1} systematic error at the shorter first overtone wavelengths.

Fitted shifts of all lines are also plotted against equivalent width and excitation potential (Fig. 8.7), confirming the conclusion in §7.3.3 that the ATMOS wavelength calibration is probably wrong by about 1.0 km s^{-1} near 5000 nm, which translates to an error of more like 2.8 km s^{-1} at the shorter wavelengths of the $\Delta\nu = 2$ lines.

Final abundance measures and isotopic ratios as defined by the weak (Table 8.2), LE (Table 8.3) and $\Delta\nu = 2$ (Table 8.4) $^{12}\text{C}^{16}\text{O}$ lines are tabulated. Errors in ^{12}C abundances are given by single standard deviations within individual $^{12}\text{C}^{16}\text{O}$ line lists. As per Barlow (2003), total standard deviations in isotopic abundances are derived by the addition in quadrature of standard deviations in the two individual contributing line lists: isotopomeric and relevant $^{12}\text{C}^{16}\text{O}$. Similarly, $^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ individual standard deviations are summed in quadrature to estimate the error in the derived bulk C abundance. Error in each isotopic ratio was computed as the difference in ratio that would result were both the ^{12}C and isotopic abundance to differ from their derived values by a single standard deviation. Overall results by the different indicators in 3D are summarised in Table 8.5.

8.5 The Solar C Abundance

The absence of significant trends in 3D model abundances over the primary (weak) and overtone ($\Delta\nu = 2$) line lists (Figs. 8.2 and 8.4), as well as the similarity of the resulting average abundances ($\log \epsilon_{\text{C}} = 8.41, 8.38$), give us confidence in the accuracy of these values. They also suggest that the 3D model is accurate in the quite high atmospheric layers in which these lines form. The agreement of abundances derived using the normal weak and overtone lines is quite an achievement, as these indicators have not generally produced consistent results. The HM model for example produces abundances differing by 0.08 dex between the two lists. It also exhibits clear trends with excitation potential for the $\Delta\nu = 2$ lines (mid-right of Fig. 8.4), further suggesting the inadequacy of its description of overtone CO. The same trends are true of MARCS, though it at least produces consistent abundances between the two line lists. That the 1DAV model abundances in these two cases are much closer to the 3D results, though still not quite as low, suggests that the primary cause of the improvement in 3D is in this case the mean temperature structure, with a secondary role played by temperature inhomogeneities.

The same success was not seen in LE results, where a striking trend with equivalent width is present in the 3D output (top left of Fig. 8.3). The reason for this is very likely the larger range of formation depths of these lines and increasing inadequacies of the 3D model atmosphere in higher layers. The weaker of the LE lines can be seen to produce abundance measures very close to the primary and overtone results, as they form at similar heights (cf. Fig. 8.1). However, the derived abundance increases with greater equivalent width and line formation height, resulting in an average abundance quite a bit higher than the primary or overtone diagnostics.

A number of reasons could be postulated for this discrepancy. The failure of the chemical equilibrium approximation (ICE) with height in the atmosphere would mean that CO density was being overpredicted in the models, producing stronger lines than otherwise would result from a particular abundance. Hence, less abundance would be required to reproduce a given line profile than in the non-ICE case, not more as is seen here. The breakdown of LTE at height in the atmosphere could possibly cause overestimated abundances here, though it seems unlikely given the repeated conclusion that CO lines form in LTE (Ayres & Wiedemann 1989; Uitenbroek 2000b). Another possibility could

$^{12}\text{C}^{16}\text{O}$ List	Weak	LE	$\Delta\nu = 2$	Adopted	Terrestrial
$\log \epsilon_{\text{C}}$	8.41 ± 0.02	8.49 ± 0.05	8.38 ± 0.02	8.40 ± 0.04	
$^{12}\text{C}/^{13}\text{C}$	$95.4^{+5.7}_{-5.4}$	$115.5^{+14.0}_{-12.5}$	$89.0^{+5.6}_{-5.3}$	$93.8^{+8.0}_{-7.6}$	$92.5^{+7.6}_{-6.5}$
$^{16}\text{O}/^{18}\text{O}$	532^{+43}_{-40}	644^{+86}_{-76}	496^{+42}_{-38}	523^{+60}_{-55}	487^{+36}_{-31}

Table 8.5: Summary of carbon abundances and isotopic ratios produced with the 3D model by the three different $^{12}\text{C}^{16}\text{O}$ line lists, as well as the adopted values. Note the poor agreement of the LE results with the other two, reflecting the trend seen in Fig. 8.3. Adopted values were calculated via 3:0:1 weightings of the weak:LE: $\Delta\nu = 2$ lists.

be that temperature contrast in the upper layers of the model is too low, as an increase in this contrast would produce lower temperature cool regions, which contribute more to increasing line strength than hotter regions would to decrease it, due to the increase in CO and the nonlinear temperature dependence of line formation. However, this could not be the explanation as the success of the Phase 2-v16 model in the previous study indicated that in fact there was *too much* temperature contrast high in the atmosphere, given that the intergranular lanes were found to be too warm at height³.

Also possible is that the velocity structure of the upper atmosphere is slightly incorrect in the 3D simulations. The MARCS model exhibited a similar equivalent width trend in implied abundances to the 3D model for the LE lines, also suggesting problems in its upper layers. In order to test this velocity hypothesis therefore, the strongest LE line (2-1 P2, see Table B.5) was recomputed using the MARCS atmosphere with increased and decreased microturbulences, as a decrease in derived abundance would indicate that the trend was due to velocity defects. When this test was performed, altered microturbulences did not reduce the derived abundance, implying that the trend was not due to the velocity structure in the 3D model. A similar test was performed with different collisional damping parameters (γ) in case this was the cause for the trend, with the same result: No improvement. One remaining possibility for the pronounced trend seen in the 3D LE results is that the mean temperature structure at height is slightly too high, causing a reduction in line strength for a given abundance and conversely, increased abundances for given line strengths. Such a conclusion would be consistent with the finding of the bisector studies of Chapter 7, so it seems most likely that this is the cause for the poor performance of the 3D model in the case of the LE lines. Based upon the previous study, the temperature overprediction seems to be in the intergranular lanes rather than the granules. This is also consistent with the lack of trend but higher average abundance indication by the 1DAV model, as the horizontal averaging would smear out the effects of overly hot intergranular lanes at height but produce higher abundances overall due to the complete absence of temperature heterogeneities.

The Phase 3-82 model of the previous chapter was trialled on the LE and weak $^{12}\text{C}^{16}\text{O}$ lines to see if agreement could be improved, and also to check that the newer model did not produce significantly different abundances where the older model was thought to be accurate (i.e. the weak lines). Derived abundances in both cases were approximately 0.03 dex larger, consistent with the effect of low resolution upon abundance determination found by Asplund et al. (2000a). We hence conclude that for abundance measures, the (Ch. 7 Phase 1) hydrodynamical simulation used in this study is no less valid than the

³remembering from §3.3.1 that high in the atmosphere, the granulation contrast reverses and intergranular lanes are warmer than granules.

later (Ch. 7 Phase 3-82) version of the code. The lack of improvement in LE lines with the lower-resolution model suggests that if the poor performance in the LE list is due to temperature overprediction in high layers, then the overprediction is not significantly compensated for by the resolutional temperature reduction in this model, as it partially appeared to be in the case of the strong $^{12}\text{C}^{16}\text{O}$ bisectors. The temperature reduction seen in the low resolution model was essentially coincidental, not based on any physical solution to the underlying cause(s) of temperature overprediction in the highest layers of the hydrodynamical simulations. Hence, it is not surprising that two different physical symptoms of the overprediction (i.e. the bisectors and the LE list abundances) would be affected differently by the unphysical impact of reduced resolution. As also stated in the previous chapter, the uppermost temperature structure of even the Phase 3-82 model might be slightly too warm.

Despite the poor performance of the 3D model in the LE list, none of the 1D models managed to derive much better agreement between these and the weak $^{12}\text{C}^{16}\text{O}$ lines (which are regarded as the best CO indicators of carbon abundance). In the sense of the LE lines' disagreement with other diagnostics, the 3D model simply presented no improvement, rather than any loss in performance over HM and MARCS. In all three diagnostics, the carbon abundance in 3D is considerably lower than indicated by HM or MARCS, as has generally been found for other species (e.g. Asplund et al. 2000c; Asplund 2000; Asplund et al. 2004c). As explained in Chapter 5, this is a general consequence of extending atmospheric simulations to three dimensions, due to the permission of temperature heterogeneities and the nonlinear temperature dependence of line formation. That all three sets of $^{12}\text{C}^{16}\text{O}$ lines continued to display this effect is a positive comment on the accuracy and consistency of the 3D model, especially given the past difficulties with 1D analyses of CO lines (Grevesse et al. 1995).

Given the relative performance of the different $^{12}\text{C}^{16}\text{O}$ line lists and their previously recognised suitability for carbon abundance determination, for the final analysis weak lines were given a weighting of 3, $\Delta\nu = 2$ lines a weighting of 1 and LE lines no weighting at all. Hence, on the basis of the lines measured in this study, the final carbon abundance arrived at is

$$\log \epsilon_{\text{C}} = 8.40 \pm 0.04$$

The final error is taken to encompass the total range of stated errors in the union of the weak and $\Delta\nu = 2$ results. That is, the adopted abundance ($\log \epsilon_{\text{C}} = 8.40$) is 0.04 dex higher than the abundance indicated by the $\Delta\nu = 2$ lines minus a standard deviation ($\log \epsilon_{\text{C}} = 8.36$), and 0.03 dex lower than the abundance indicated by the weak lines plus a standard deviation ($\log \epsilon_{\text{C}} = 8.43$), with the final error taken to be the greater of these differences ($\Delta\epsilon = 0.04$). This is considered preferable to again summing the statistical errors in quadrature of the individual weak and $\Delta\nu = 2$ carbon abundances, as systematic errors such as the model atmosphere, atomic data and measured equivalent widths no doubt dominate over the statistical errors seen within line lists.

The adopted abundance is in excellent agreement with the $\log \epsilon_{\text{C}} = 8.39 \pm 0.05$ of Asplund et al. (2004a), which was based on very different indicators (see §3.4.7). The current figure therefore firms our belief in the accuracy of *both* carbon results *and* the 3D model atmosphere. Given the height of formation of the CO lines, this result is a remarkable success for the 3D model. The new carbon abundance constitutes a major reduction from the currently accepted Grevesse & Sauval (1998) value of $\log \epsilon_{\text{C}} = 8.52 \pm 0.06$, not

to mention a multitude of even higher earlier estimates (e.g. Harris et al. 1987).

8.6 The Solar $^{12}\text{C}/^{13}\text{C}$ and $^{16}\text{O}/^{18}\text{O}$ Ratios

The abundances produced by the individual $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ lines in 3D (the left of Figs. 8.5 and 8.6) show no significant wavelength, equivalent width or excitation potential dependence, hence illustrating no inadequacies in the model. This is also more or less the case for the 1D simulations of the $^{13}\text{C}^{16}\text{O}$ lines (the right of Fig. 8.5) but not the $^{12}\text{C}^{18}\text{O}$ lines, where trends with equivalent width and excitation potential are evident in the HM and MARCS results (the right of Fig. 8.6). The two trends are explicitly linked, as the higher excitation lines form lower and therefore have smaller equivalent widths, so it is no surprise that one trend exists in equivalent width and the opposite is seen in excitation potential. These trends would seem to indicate the superiority of the 3D model in the description of the very weak $^{12}\text{C}^{18}\text{O}$ lines.

The derived isotopic ratios in Tables 8.2-8.4 using the different model atmospheres show a very strong separation between 3D and 1D results. This is most curious, and evidently constitutes a very important improvement in the move from one to three modelling dimensions. This fact is highlighted in particular by the stark difference between 3D and 1DAV results in all three tables. The reason for the greater decrease in isotopic abundances than the carbon abundance in 3D (at least in the case of the weak $^{12}\text{C}^{16}\text{O}$ lines) is that the isotopomeric lines used are actually over 20% more temperature sensitive than the weak $^{12}\text{C}^{16}\text{O}$ lines (Grevesse & Sauval 2004). This means that the heterogeneous temperature structure of the 3D simulations (which is responsible for reduced abundances normally) has a greater decreasing effect upon the isotopic lines and therefore ^{13}C and ^{18}O abundances than it does upon the derived carbon abundance. Because of this differential temperature sensitivity, the horizontal averaging implicit in 1D models means that they have difficulty reproducing the correct solar isotopic ratios. The temperature sensitivity of the LE and $\Delta\nu = 2$ lines is unclear, though it is suspected that the difference between 3D and 1D results in the case of these lists has a similar cause to that seen in the weak list.

Because each $^{12}\text{C}^{16}\text{O}$ list produced different carbon abundances and each was compared to the same $^{13}\text{C}^{16}\text{O}$ and $^{12}\text{C}^{18}\text{O}$ results, significantly different 3D isotopic ratios were obtained. However, the LE ratios can be discarded out of hand due to the already established invalidity of the LE carbon abundance. In the derivation of the final isotopic ratios, the $\Delta\nu = 2$ ratios were given a low weighting in the same manner as in the calculation of the final carbon abundance (i.e. one third of the weighting afforded the weak ratios). Hence, the adopted isotopic ratios are:

$$\begin{aligned} ^{12}\text{C}/^{13}\text{C} &= 93.8^{+8.0}_{-7.6} \\ ^{16}\text{O}/^{18}\text{O} &= 523^{+60}_{-55} \end{aligned}$$

Errors are this time taken as the sum in quadrature of statistical errors in the weak and $\Delta\nu = 2$ results. This is because it is assumed that the systematic errors discussed as relevant to the carbon abundance in §8.5 effect all the lines considered for the adopted isotopic ratios equally, so need not be included in final *ratio* errors. This assumption is based on fact that the isotopic, weak and $\Delta\nu = 2$ lines all reflect essentially the same line formation processes, as they form at the same height in the atmosphere.

Using the HM model, Harris et al. (1987) produced ratios of $^{12}\text{C}/^{13}\text{C} = 84 \pm 5$ and

$^{16}\text{O}/^{18}\text{O} = 440 \pm 50$. In comparison, our own HM results (weighted amongst the lists in the same manner as the 3D ratios) were $^{12}\text{C}/^{13}\text{C} = 71.7_{-6.2}^{+6.6}$ and $^{16}\text{O}/^{18}\text{O} = 363_{-48}^{+52}$. The difference in HM results between the two studies evidently reflects the improved observations, line lists and molecular data used in the present work⁴. However, the effect of these improvements is to reduce the ratios, whereas the adopted ratios calculated in 3D are significantly greater than those previously found. Therefore, the difference between old and new *adopted* ratios primarily reflects the shift from 1D to 3D modelling, with the effects of this shift in fact partially nullified by improved input data. The results presented here are hence more valid than those of the past, and constitute a very significant upwards revision of the ratios.

The $^{12}\text{C}/^{13}\text{C}$ ratio found is in excellent agreement with the Rosman & Taylor (1998) terrestrial value of $92.5_{-6.5}^{+7.5}$. This ratio corresponds to a $\delta^{13}\text{C}$ value of -14_{-77}^{+87} without taking into account the terrestrial uncertainty inherent in this scale, in agreement with some of the widely variable lunar regolith measures discussed by Wiens et al. (2004). Given this new high value for $^{12}\text{C}/^{13}\text{C}$, the enrichment of the ISM over the Sun's lifetime indicated by Langer & Penzias (1993) with their local ISM value of 62 ± 4 becomes even more pronounced. This would therefore seem to indicate an increased amount of galactic chemical evolution or isotopic inhomogeneity within our galaxy (through which the solar system has moved in its lifetime) than previously thought.

The derived $^{16}\text{O}/^{18}\text{O}$ abundance is certainly reasonably close to the terrestrial ratio of 487_{-31}^{+36} (Rosman & Taylor 1998), though a little further removed from the telluric value than the derived $^{12}\text{C}/^{13}\text{C}$ ratio. Whether this difference is meaningful at all is impossible to say given the error bounds of the solar and terrestrial values. Indeed, the corresponding $\delta^{18}\text{O}$ value of -69_{-96}^{+109} (where the terrestrial error in the scale is not accounted for) is tantalisingly close to the $\delta^{18}\text{O} = -50$ prediction of the self-shielding model discussed in §5.3 (Yurimoto & Kuramoto 2004; Yin 2004). However, considering

- the large errors evident when our result⁵ is expressed in the geological fractionation scale
- the errors inherent in the terrestrial values and therefore the scale itself
- the fact that no error bars are stated in the self-shielding prediction of $\delta^{18}\text{O}$ (Yurimoto & Kuramoto 2004)

it is impossible to legitimately conclude that the solar $\delta^{18}\text{O}$ value is or is not terrestrial, or does or does not bear out the self-shielding prediction. We hence conclude only that the derived ratio disagrees with neither the terrestrial abundance or the self-shielding model for solar system formation.

⁴Derived equivalent widths for the few lines common to the two studies showed quite large differences in some cases.

⁵Or any other result, for that matter.

Conclusions

Following three phases of work (Chapter 7) employing a number of variants of the standard 3D model atmosphere (Asplund et al. 2000b), observed strong CO line profiles and bisectors were reproduced quite well. This is the most successful modelling of CO line formation in the solar atmosphere to date. Evidence for the presence of a COmosphere was found, existing predominantly below a height of 700 km. This result does not preclude the existence of cool gas higher in the atmosphere, but simply puts an upper limit on the extent of *significant* CO concentration.¹ Whether this height of 700 km or the ~ 1000 km suggested by Ayres (2002) should define the ‘top’ of the COmosphere is open for debate. The characteristic temperature of the modelled COmosphere responsible for the successful reproduction of CO spectral features was 3900–4100K, warmer than the 3500K predicted by Ayres. The 3500K figure was based upon a COmosphere extending beyond 700 km though, where gas would naturally be cooler than seen in this study. However, owing to the inhomogeneity permitted by three-dimensional modelling, evidence was found even at heights of 700 km for persistent gas temperatures as low as 3700K, and intermittent temperatures as low as 2000K.

The successful modelling of strong CO lines in Chapter 7 was attributable to both an improved version of the Stein-Nordlund code (Trampedach 2004) and fortuitous resolutional effects. Despite the improved code, evidence was found for a slight overprediction of temperature in the uppermost intergranular regions in general by the 3D model atmospheres, and a correspondingly overpredicted mean temperature structure. This conclusion was supported by poor performance of the 3D model in abundance determinations using the strongest of the LE (low excitation) CO lines in Chapter 8. It should be noted however that the model’s temperature structure is only very slightly inaccurate at extreme height; other successful abundance measurements (Chapter 8) using CO lines themselves formed fairly high (though not quite so high as many of the LE or strong lines) demonstrate that except in the very highest layers, the 3D model temperature structure can be considered highly accurate.

Solar abundance determinations using CO lines performed in Chapter 8 produced a carbon abundance of $\log \epsilon_{\text{C}} = 8.40 \pm 0.04$, and isotopic ratios of $^{12}\text{C}/^{13}\text{C} = 93.8^{+8.0}_{-7.6}$ and $^{16}\text{O}/^{18}\text{O} = 523^{+60}_{-55}$. These results represent a significant improvement over those of the past due to the combination of a state-of-the-art convective 3D model atmosphere, updated atomic data, better line lists and more accurate observations. The carbon abundance is in excellent agreement with the recent findings based upon entirely different indicators of Asplund et al. (2004a), indicating that the past problems with CO-derived abundances

¹‘Significant’ might be defined either by the influence of the gas upon disc centre profiles or the non-ICE downturn in CO concentration seen by Asensio Ramos et al. (2003), Fig. 4.5.

have been solved. The $^{12}\text{C}/^{13}\text{C}$ ratio is in excellent agreement with the telluric value (Rosman & Taylor 1998). The $^{16}\text{O}/^{18}\text{O}$ ratio found also does not contradict the telluric value (Rosman & Taylor 1998), though nor does it contradict that predicted by the self-shielding model of solar system formation (Yurimoto & Kuramoto 2004).

9.1 Future Directions

Following these findings, the most obvious follow-up study that could be performed is the generation of a full $200 \times 200 \times 82$ version of the Chapter 7 Phase 3-82 model. The strong CO lines could then be modelled using this new atmosphere, and the relative effects of resolution and model improvements upon the results of §7.3 determined with certainty. There is no doubt that even the latest version of the code could use some work in improving the emergent temperature structure in the uppermost layers, and this type of investigation would provide more clues as to how this might be achieved. Such efforts to correct the slightly anomalous temperature structure that caused problems in modelling the strong and LE line lists present a further avenue for extending this work. However, given that many of the assumptions on which the model atmospheres are based approach the limits of their applicabilities in these high layers (e.g. LTE, opacity binning, ignoring magnetic fields), it is not at all clear how or even if this might realistically be achieved under current computational constraints.

An interesting extension would be the investigation of the centre to limb behaviour of the CO lines. This would provide another probe of the temperature structure in the upper regions of the model and actual atmospheres, and it would be very useful to compare such results with those of the two studies presented here. The only thing preventing such an extension at this stage is the availability of off centre observations in the cores of the CO lines; the models are already fully equipped to produce synthetic versions of these spectra, but the observational data is lacking. In fact, a request for such data was made to Han Uitenbroek (who it was decided would be the most likely person to have performed such observations) for inclusion in this thesis along with corresponding model output, but he unfortunately had no appropriate observations available at this time.

Yet another possible extension of this work would be to calculate CO number densities in the radiative transfer calculations without the assumption of instantaneous chemical equilibrium (ICE). This would prove useful both in terms of improving the realism of the simulations and as a comparison with similar efforts of Asensio Ramos et al. (2003) using the Carlsson-Stein model. The improved realism would be best evaluated and borne out most in the centre to limb behaviour of the CO lines, so such a followup might be performed together with the aforementioned off centre observations and modelling. Asensio Ramos et al. (2003) indicated that they proposed to do something similar to this in the near future, though they seem to intend to go so far as to include non-ICE evolution and the resulting effects upon molecular cooling in the *hydrodynamical* simulations. This would seem a very difficult task, especially seeing as molecules are not only currently treated in ICE but are not even included in the equation of state in the hydrodynamical code, so the study would appear unlikely to eventuate soon.

In terms of abundance measurements, there are many, many more CO lines and relevant molecular data available for testing with the 3D model. A comprehensive study of the abundances produced by the myriad different compilations of CO lines that could be investigated would certainly be an interesting one to see the results of, though one suspects possibly less so to perform. Likewise, the rederivation of solar abundances for the many

trace elements not yet investigated with the 3D models is an obvious pathway for future work, though likely also somewhat tedious. However, these studies should certainly be carried out, as the results for other elements and their isotopes will no doubt prove useful, as the $^{16}\text{O}/^{18}\text{O}$ ratio is for example, for various other fields. Indeed, perhaps the best way to drive this continued progression is increased collaboration with other astronomers, astrophysicists and planetary scientists, and a focus upon the elements and isotopes most useful to them.

The exclusive focus of this thesis has been the Sun, though at the current time the 3D models are being applied as much to the analysis of other stars as to our own. The results presented here will hence also serve as a useful reference point for another logical progression: Analysis of CO in other stars using the same techniques. As a final comment, the enduring request of the solar or stellar spectroscopist (e.g. Grevesse et al. 1995; Kurucz 2002) for yet more atomic and molecular data, as well as higher-resolution spectra, should continue to be heeded and drive further work in these areas.

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Computational Appendix

The following is an inventory of the major programs written or altered for the purposes of this thesis. Programs written in their entirety are described in §A.1, whilst the changes made to existing codes are listed in §A.2. In addition to those listed, assorted lesser one-off and utility programs were also written. This inventory acts both as an aide for describing the methods employed in Chapters 6-8 as well as a brief indication of the computational undertakings involved in this work. It is not intended as complete documentation of these undertakings, and as such does not include any code listings. For readers interested in examining the codes used, repeating or extending sections of this work, all programs are available upon request from pat@mso.anu.edu.au or martin@mso.anu.edu.au.

A.1 Programs Written

`name` (language) (*arguments/keywords*)

`abunplot` (IDL) (*nlines*, *infile1*, *infile2*, *plotcode*, *baseabun1*, *baseabun2*, *yvals*, *whatIsIt*, *ps*, *mK*)

Reads in abundances indicated by individual lines in *infile1* (and optionally *infile2*), then produces a plot against equivalent width, excitation potential or wavelength according to *plotcode* (e.g. Figs. 8.2-8.4). Converts stored abundance differences to actual abundances by adding *baseabun1* (and optionally *baseabun2*). Produces screen or PostScript output depending on *ps*, accepts either pm or mK stored equivalent widths depending on *mK* and labels y-axis with *whatIsIt* over the range *yrange*.

`atmos_read` (IDL) (*lambdaMin*, *lambdaMax*, *truncatedSpectrum*, *plot*)

Reads in ATMOS header data and plots spectrum (if *plot* is set) retrieved using `spec_read`. Spectrum produced runs from *lambdaMin* to *lambdaMax*, and is returned in the variable *truncatedSpectrum*.

`beerbroad` (IDL) (*wavelength*, *spectrum*, *N*, *hwfz*, *cont*, *fine*)

Performs BNA (Beer-Norton apodization) of the vector *spectrum* over the wavelength vector *wavelength*, which may be in frequency, wavenumber, wavelength or Doppler velocity units. Constructs apodizing functions with characteristic resolution *hwfz* (presuming the same units as *wavelength*) and performs convolution. *N* determines whether the convolving function is a traditional sinc, weak, medium or strong Beer-Norton ILS.

`bulk_CO` (IDL) (*searchWidth*, *outputTable*, *bisectors*)

Searches a width *searchWidth* about line centres returned from `read_colines` for absorption lines in the ATMOS spectrum using `atmos_read`. Computes shifts, centres and bisectors (using `line_analyse`) for all lines returned by `read_colines`. Plots all bisectors and returns *outputTable* of lab wavelength, observed wavelength and shift in both nm and ms^{-1} , as well as array of pointers (*bisectors*) to arrays containing individual line bisectors. Also outputs bisector arrays to data files for later use by `multiprofile`.

`difplotter` (IDL) (*linefile*, *fileExtension*, *species*)

Reads in individual bisector difference files produced by `multiprofile`, as specified by *linefile*, *fileExtension* and *species* and plots all differences on the same set of axes (e.g. Figs. 7.2, 7.5 and 7.7).

`DopplerLtoV` (IDL) (*lambdaObserved*, *lambdaReference*)

Returns Doppler velocity array of wavelengths in *lambdaObserved*, relative to *lambdaReference*.

`DopplerVtoL` (IDL) (*velocity*, *lambdaReference*)

Returns wavelength array of Doppler velocities in *velocity*, relative to *lambdaReference*.

`line_analyse` (IDL) (*outputarray*, *plot*)

Calculates line centre and bisector for a single line via cubic spline interpolation. First interpolates to finer wavelength values, then finds line centre, splits line in two at the centre, interpolates to finer intensity values and finally sticks line back together. Bisector is then calculated as midpoint of wavelength values of opposite sides of the line having the same intensity. Input array (*outputarray*, though redimensioned and also used for bisector output) must consist of just one line and wings. If *plot* is set, plots interpolated line and bisector. Interpolation resolution in both wavelength and intensity is internally configurable.

`obs_line` (IDL) (*lambdaMin*, *lambdaMax*)

Uses `atmos_read` and `line_analyse` to plot a single line and bisector from the ATMOS spectrum in the wavelength range [*lambdaMin*, *lambdaMax*].

`spec_read` (IDL) (*outputarray*, *assorted ATMOS header variables*)

Uses ATMOS header variables passed as input to extract and scale ATMOS spectrum from ATMOS data files according to instructions in Irion et al. (2002a). Returns *outputarray* containing spectrum.

`trends` (IDL) (*searchWidth*, *graphtype*)

Reads lines using `read_colines`, extracts widths *searchWidth* from the ATMOS spectrum about line centres using `atmos_read`, then determines line centres, shifts and bisectors using `line_analyse`. Outputs one data file containing core wavelength, shift, depth, strength and lower excitation potential for each line. So named because it also produces a PostScript plot of one of these quantities against another, depending upon the value of *graphtype*.

A.2 Programs Altered

chi2 (IDL)

Allowed inclusion of errors in data upon which χ^2 measure was performed, permitting appropriate weighting of individual data points in calculation of χ^2 . Also altered to output number of points fit is made upon, facilitating reduction of initial χ^2 measure.

multiprofile (IDL)

Over 50% of the line profile display program `profile` generally used to reduce the 3D hydrodynamic model output was rewritten. Provision was added to operate upon an entire line list via the use of `read_colines`, outputting plots to screen or successive PostScript files along with a summary data file containing reduced χ^2 values, depths, strengths and shifts for each line. The ability to incorporate ATMOS data in the calculations and output was included with the use of `atmos_read` and altered `read_prof` and `read_obs`. The provision for profile fitting in abundance and wavelength shift variables by minimisation of the χ^2 statistic (using `chi2`) was added. An ordering bug in the existing convolution of synthetic lines with macroturbulent or instrumental profiles was identified and remedied. This made such convolutions compatible with simultaneous abundance determination using either profile or equivalent width fitting. Assorted cosmetic alterations were also made to the output plots. Finally, observed and synthesised bisector difference interpolation, calculation and output was included in the program design, allowing the function of `difplotter`.

rayt (FORTRAN)

Altered to include mass and opacity scalefactors in radiative transfer simulation line opacity calculations, according to §8.2. Scalefactors were provided by `trline`.

read_colines (IDL)

A bug incorrectly interchanging J quantum numbers and statistical weights of rotation-vibration initial energy levels was remedied. Correct calculation of final J quantum numbers via the analysis of transition branch was also included, and the corresponding entries in the master line database corrected.

read_obs (IDL)

Altered to allow input of bisector data files produced by `bulk_CO`. In particular, the provision for input of error data associated with bisectors was greatly improved and the manner of their display made more flexible.

read_prof (IDL)

Altered to allow reading of ATMOS profiles using `atmos_read`.

sincbroad (IDL)

A bug was fixed in sinc function generation where input spectral resolution was incorrectly doubled and treated as if it were comparable to the full width half maximum of the convolving Gaussian used in macroturbulent broadening. The bug appears to have arisen when the routine was first adapted in 1992 from the equivalent macrobroadening convolution algorithm. Changes were made to this program following the identification of the bug only for backwards compatibility, given that **sincbroad** was superseded by **beerbroad** anyway.

trline (FORTRAN)

Altered to include the reading of an extra input file in initialisation of the radiative transfer simulations. Contents of the input file (mass and opacity scalefactors) were made available to **rayt**.

Line Lists

Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)
4752.1533	5-4 R19	-2.9376	1.130
4741.2775	2-1 P2	-4.3324	0.267
4739.9862	6-5 R31	-2.6541	1.521
4726.7267	1-0 P7	-4.0876	0.013
4719.1825	4-3 R15	-3.1271	0.843
4718.1039	7-6 R49	-2.3921	2.093
4717.6910	1-0 P6	-4.1536	0.010
4715.7219	2-1 R0	-4.6309	0.266
4696.2029	5-4 R28	-2.7701	1.229
4679.3794	5-4 R31	-2.7255	1.270
4666.9654	3-2 R14	-3.2739	0.577
4663.4526	5-4 R34	-2.6846	1.316
4638.8782	5-4 R39	-2.6236	1.400
4634.2564	5-4 R40	-2.6123	1.418
4627.2312	6-5 R58	-2.3744	2.066
4619.1075	6-5 R61	-2.3517	2.146
4614.8044	4-3 R32	-2.8007	1.031
4603.5454	6-5 R68	-2.3028	2.347
4600.7586	5-4 R48	-2.5304	1.579
4584.7513	4-3 R38	-2.7243	1.129
4584.3568	3-2 R27	-2.9931	0.705
4582.1879	2-1 R18	-3.3375	0.346
4510.9808	2-1 R30	-3.1158	0.485
4480.4509	2-1 R36	-3.0348	0.579
4457.5278	2-1 R41	-2.9763	0.670
4450.3204	1-0 R31	-3.3956	0.236
4398.4026	1-0 R42	-3.2592	0.428
4341.8489	1-0 R58	-3.1113	0.807
4339.0480	1-0 R59	-3.1034	0.834
4336.3331	1-0 R60	-3.0957	0.862
4333.7041	1-0 R61	-3.0880	0.891

Table B.1: Strong $^{12}\text{C}^{16}\text{O}$ line list used for the Chapter 7 study, consisting of 31 lines. Provided by Grevesse & Sauval (2004), who calculated $\log gf$ data from Goorvitch & Chackerian (1994).

Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)
6162.3540	1-0 P98	-3.046	2.242
6112.9978	1-0 P96	-3.053	2.154
4309.8852	1-0 R109	-2.842	2.750
4306.7253	1-0 R107	-2.848	2.654
4303.9460	1-0 R105	-2.857	2.560
4301.5437	1-0 R103	-2.867	2.467
4299.5151	1-0 R101	-2.873	2.376
4298.6396	1-0 R100	-2.879	2.331
4297.8564	1-0 R99	-2.883	2.286
4297.1649	1-0 R98	-2.889	2.242
6329.1932	2-1 P101	-2.742	2.619
6251.2034	2-1 P98	-2.752	2.486
6225.7984	2-1 P97	-2.755	2.443

Table B.2: Weak $^{12}\text{C}^{16}\text{O}$ line list used for the Chapter 8 study, consisting of 13 lines. Provided by Grevesse & Sauval (2004), who calculated $\log gf$ data from Goorvitch & Chackerian (1994).

Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)
4542.4821	3-2 R62	-2.658	1.380
4539.7468	2-1 R46	-2.963	0.745
4535.7888	2-1 R47	-2.951	0.766
4528.1342	2-1 R49	-2.932	0.809
4513.8671	2-1 R53	-2.896	0.901
4501.6474	1-0 R42	-3.297	0.409
4497.3756	1-0 R43	-3.286	0.429
4493.1896	1-0 R44	-3.275	0.448
4486.8117	2-1 R62	-2.827	1.132
4481.1460	1-0 R47	-3.245	0.511
4474.7857	2-1 R67	-2.790	1.275
4457.1692	2-1 R77	-2.726	1.591
4456.0218	1-0 R54	-3.182	0.671
4454.6795	2-1 R79	-2.714	1.660
4452.7709	1-0 R55	-3.173	0.695
4449.6042	1-0 R56	-3.165	0.720

Table B.3: $^{13}\text{C}^{16}\text{O}$ line list used for the Chapter 8 study, consisting of 16 lines. Provided by Grevesse & Sauval (2004), who calculated $\log gf$ data from Goorvitch & Chackerian (1994).

Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)
5243.7159	1-0 P43	-3.370	0.427
5127.5809	1-0 P34	-3.462	0.269
5044.7281	1-0 P27	-3.556	0.171
5033.4006	1-0 P26	-3.572	0.159
4478.6546	1-0 R50	-3.219	0.574
4486.1030	1-0 R48	-3.237	0.530
4482.3365	1-0 R49	-3.228	0.552
5154.8355	2-1 P31	-3.205	0.482
5130.8774	2-1 P29	-3.233	0.455
5084.5153	2-1 P25	-3.293	0.405
5336.4145	3-2 P40	-2.932	0.879
5270.2261	3-2 P35	-2.987	0.796
5190.1890	4-3 P23	-3.039	0.891
5167.4916	4-3 P21	-3.077	0.871
5393.2644	5-4 P34	-2.788	1.278

Table B.4: $^{12}\text{C}^{18}\text{O}$ line list used for the Chapter 8 study, consisting of 15 lines. Provided by Grevesse & Sauval (2004), who calculated $\log gf$ data from Goorvitch & Chackerian (1994).

Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)
4916.3051	5-4 P1	-4.2733	1.044
4898.5440	5-4 R0	-4.2716	1.043
4881.2454	5-4 R2	-3.7932	1.045
4864.4047	5-4 R4	-3.5686	1.048
4934.5350	5-4 P3	-3.7986	1.046
4943.8275	5-4 P4	-3.6737	1.048
4962.7720	5-4 P6	-3.4989	1.053
4862.5943	4-3 P2	-4.0625	0.789
4871.6187	4-3 P3	-3.8861	0.790
4880.7591	4-3 P4	-3.7620	0.792
4836.2087	4-3 R0	-4.3615	0.787
4827.6411	4-3 R1	-4.0595	0.788
4801.2476	3-2 P2	-4.1805	0.530
4715.7219	2-1 R0	-4.6478	0.266
4741.2775	2-1 P2	-4.3497	0.267

Table B.5: Low excitation (LE) $^{12}\text{C}^{16}\text{O}$ line list used for the Chapter 8 study, consisting of 15 lines. Provided by Grevesse & Sauval (2004), who calculated $\log gf$ data from Goorvitch & Chackerian (1994).

Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)	Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)	Wavelength (nm)	Transition	$\log gf$	Excitation Pot. (eV)
2363.1249	2-0 P 7	-6.2233	0.013	2297.7720	2-0 R65	-5.0410	1.009	2345.4162	3-1 R17	-5.2660	0.338
2368.0105	2-0 P 9	-6.1192	0.021	2298.3892	2-0 R66	-5.0315	1.039	2344.0666	3-1 R18	-5.2396	0.346
2378.3082	2-0 P13	-5.9706	0.043	2408.3440	3-1 P13	-5.4868	0.309	2342.7584	3-1 R19	-5.2140	0.355
2398.0498	2-0 P20	-5.7986	0.100	2413.8559	3-1 P15	-5.4295	0.322	2341.4918	3-1 R20	-5.1904	0.365
2401.0522	2-0 P21	-5.7799	0.110	2416.6808	3-1 P16	-5.4034	0.330	2339.0825	3-1 R22	-5.1457	0.385
2404.1007	2-0 P22	-5.7620	0.120	2422.4694	3-1 P18	-5.3565	0.346	2337.9399	3-1 R23	-5.1244	0.396
2437.1831	2-0 P32	-5.6216	0.251	2434.6085	3-1 P22	-5.2790	0.385	2336.8385	3-1 R24	-5.1035	0.407
2459.3740	2-0 P38	-5.5591	0.352	2437.7618	3-1 P23	-5.2620	0.396	2330.2818	3-1 R31	-4.9747	0.499
2471.1542	2-0 P41	-5.5317	0.408	2457.6960	3-1 P29	-5.1739	0.471	2329.5096	3-1 R32	-4.9626	0.514
2475.1846	2-0 P42	-5.5229	0.428	2461.1901	3-1 P30	-5.1618	0.485	2327.4396	3-1 R35	-4.9136	0.562
2491.8344	2-0 P46	-5.4908	0.512	2468.3280	3-1 P32	-5.1379	0.514	2326.2652	3-1 R37	-4.8861	0.596
2523.0648	2-0 P53	-5.4425	0.676	2471.9723	3-1 P33	-5.1261	0.530	2325.7397	3-1 R38	-4.8697	0.614
2527.7505	2-0 P54	-5.4353	0.701	2483.2111	3-1 P36	-5.0947	0.579	2324.8122	3-1 R40	-4.8447	0.651
2328.4851	2-0 R 9	-6.0241	0.021	2490.9617	3-1 P38	-5.0752	0.614	2324.4103	3-1 R41	-4.8297	0.670
2322.0848	2-0 R13	-5.8665	0.043	2498.9218	3-1 P40	-5.0570	0.651	2323.3645	3-1 R56	-4.6536	1.012
2317.7138	2-0 R16	-5.7747	0.065	2580.5013	3-1 P58	-4.9281	1.065	2326.1201	3-1 R63	-4.5834	1.206
2313.7084	2-0 R19	-5.6946	0.090	2590.7333	3-1 P60	-4.9172	1.120	2326.6855	3-1 R64	-4.5735	1.235
2310.0671	2-0 R22	-5.6253	0.120	2359.4419	3-1 R 8	-5.5901	0.283	2327.2943	3-1 R65	-4.5638	1.265
2308.9340	2-0 R23	-5.6055	0.131	2351.2311	3-1 R13	-5.3851	0.309	2329.3824	3-1 R68	-4.5346	1.357
2306.7886	2-0 R25	-5.5638	0.155	2349.7148	3-1 R14	-5.3526	0.315	2330.9940	3-1 R70	-4.5171	1.421
2305.7763	2-0 R26	-5.5452	0.167	2348.2403	3-1 R15	-5.3224	0.322	2338.0411	3-1 R77	-4.4559	1.657
2295.4058	2-0 R41	-5.3098	0.408	2346.8074	3-1 R16	-5.2933	0.330	2341.7430	3-1 R80	-4.4306	1.765

Table B.6: First overtone ($\Delta\nu = 2$) $^{12}\text{C}^{16}\text{O}$ line list used for the Chapter 8 study, consisting of 66 lines. Provided by Grevesse & Sauval (2004), who calculated $\log gf$ data from Goorvitch & Chackerian (1994).