Computing solar absolute fluxes

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Summary. Computed color indices and spectral shapes for individual stars are routinely compared with observations for essentially all spectral types, but absolute fluxes are rarely tested. We can confront observed irradiances with the predictions from model atmospheres for a few stars with accurate angular diameter measurements, notably the Sun. Previous calculations have been hampered by inconsistencies and the use of outdated atomic data and abundances. I provide here a progress report on our current efforts to compute absolute fluxes for solar model photospheres. Uncertainties in the solar composition constitute a significant source of error in computing solar radiative fluxes.

1 Introduction

The spectrum of the Sun is the outcome of the physics governing the outer layers of our star. Understanding the formation of the solar spectrum is a necessary step in order to be able to predict its variability along the solar magnetic cycle and to measure the solar surface composition. The solar spectrum at wavelengths longer than about 140 nm is variable only at the few-percent level, and given the exquisite accuracy of the solar parameters, observations of the Sun may provide the best available standard to calibrate and guide the construction of theoretical model atmospheres for late-type stars. Ultimately, our ability to predict the luminosities of other stars and entire galaxies can be tested and improved by studying the solar spectrum.

The UV part of the spectrum is of particular relevance for us, as it is closely connected to the chemistry of the Earth’s atmosphere, and the evolution of life on Earth. Astrophysically, the UV is exciting for its wealth of information: the strongest atomic lines concentrate in this spectral window, and so do ionization edges. Although the Sun is not a particularly luminous star, it shares atmospheric physics with other F-G-K late-type stars which contribute significant mass and light to distant galaxies, as shown in many of the papers included in this volume.
Perhaps the most severe difficulty to model the outer layers of the Sun is related to the existence of an 'upper atmosphere', where the time-averaged thermal gradient is reversed and a combination of high temperature and low density drives the plasma far from equilibrium conditions (see, Judge 2005 and Rutten 2007 for recent reviews). Semi-empirical time-independent models of the upper atmosphere have provided significant insight (see, e.g., the classical Vernazza, Avrett & Loesser 1981 paper). Increasingly sophisticated hydrodynamical simulations are making their way upwards into the lower chromosphere (Wedemeyer et al. 2004; Wedemeyer-Böhm et al. 2007).

Space imagery of the upper atmosphere reveals a complicated interaction of magnetic field and waves. Such images contrast with the much simpler picture that we get from optical observations of the photosphere, where the magnetic field that permeates our star causes only a small distortion from field-free conditions, and the temperature contrast of the granulation is only a few percent. Fortunately, it is possible to study the lower atmosphere independently from higher layers. In the optical and infrared the upper atmosphere is optically thin and the opacity, dominated by the H− continuum, is only superseded by metal opacity at wavelengths shorter than about 300 nm. As we move further into the UV, the rapidly increasing metal opacity shifts the spectrum formation into the lower chromosphere. The change of character is reflected in the time variability of the integrated solar spectrum, which exceeds 10 % at $\lambda \sim 140$ nm and 50 % at $\lambda < 120$ nm.

An array of empirical models that represent the different magnetic structures on the solar surface (e.g. sunspots, plage, network, etc.) needs to be considered to describe the variability of the solar spectrum throughout the solar cycle (see, e.g., Fligge, Solanki & Unruh 2000, Fontenla et al. 1999), but at $\lambda > 200$ nm, a single model is expected to be a reasonable approximation, given that the vast majority of the solar surface is typically free from regions with strong magnetic fields (what is usually referred to as the 'quiet' Sun or the internetwork).

There is an extensive literature on the comparison of calculated and observed solar UV fluxes. Most readers will remember the UV missing opacity problem, but the literature on this subject has been sparse over the last decade. We first review recent results, and then move on to describe our current efforts to improve models of the solar photosphere and compile updated opacities.

2 Anybody said 'missing' opacity?

Early studies found too much UV flux in model atmosphere calculations (Houtgast & Namba 1968, Labs & Neckel 1968, Matsushima 1968). Based on a linelist from semi-empirical calculations of atomic structure (Kurucz & Peytremann 1975), completed with literature values, Kurucz (1992) concluded that the problem was solved, but his proposal was criticized by Bell et al.
Bell, Balachandran & Bautista (2001) revisited this issue armed with updated Fe I opacity from the R-matrix calculations of Bautista (1997), concluding that the problem was significantly reduced, but still present. They found that if iron opacity was responsible for the deficit, the new data could only account for half of the missing opacity. More recently, we performed a similar study using Gaussian-averaged photoionization cross-sections from the opacity project for elements with atomic numbers 6–14 and scaled hydrogenic cross-sections for Fe I, arriving at the opposite conclusion (Allende Prieto, Hubeny & Lambert 2003a).

Independently, Fontenla et al. (1999, see also Fontenla et al. 2006) used a combination of semi-empirical models to model the solar spectrum. They noticed an opacity deficit around 410 nm. Nonetheless, the use of semi-empirical models whose temperature structure have been modified to reproduce observed fluxes, makes the discussion of absolute fluxes somewhat circular. Note also that the continuum metal opacities considered in these studies are outdated and neglect atomic iron.

There were several differences among the calculations of Balachandran et al. and ours. First of all, different model atmospheres were used: a MARCS model versus an interpolated Kurucz (1993) solar model. A different solar surface composition was adopted by the two groups. Most relevant, Balachandran et al. adopted log $\epsilon$(Mg)$=7.44$ and log $\epsilon$(Fe)$=7.55$, and we used log $\epsilon$(Mg)$=7.58$ and log $\epsilon$(Fe)$=7.50$. Our higher magnesium abundance can explain up to about 5% less flux in our calculations at 400 nm and up to 20% shortwards of 300 nm (see Section 4), but the difference between the iron abundances, although smaller, goes in the wrong direction.

Our calculations had (at least!) one prominent shortcoming: molecular opacity was neglected. We also made a mistake, including natural damping in Lα too far from the transition’s frequency. Mathematically, the natural damping contribution to the Lorentzian wings of Lα is strong enough to contribute very far, even into the optical. Natural damping in Lyman alpha far from the transition frequency becomes in fact Rayleigh scattering, and should be treated as such.

The opacity deficit, if any, has not been clearly linked to photoionization of atomic iron, and the solar photospheric abundances of several major elements have been systematically reduced over the last few years (see Asplund 2005, Asplund, Grevesse & Sauval 2005). It is time to take a closer look at this issue.
3 Revisiting the problem: opacities, equation of state, chemical composition and model atmospheres

The problem of atmospheric structure, regardless of geometry, is intrinsically coupled to the chemical composition of the star. The relevant atomic and molecular opacities need to be accounted for, not only to predict accurately the spectrum shape, but also to describe properly the energy balance, equation of state and, ultimately, the atmospheric structure (see the paper by Hubeny in this volume). The chemical composition of the solar atmosphere, in turn, is determined from spectral synthesis calculations based on a model atmosphere computed for a given composition. Thus, abundances, opacities, equation of state, and model atmospheres are intrinsically coupled: changing one of these elements in isolation may be meaningless.

Below, we briefly describe the main updates that we are implementing in our calculations.

3.1 Abundances

Over the last 7 years, a number of spectroscopic investigations of the solar chemical composition have significantly modified the standard values generally adopted for the solar photosphere. The largest updates affect some of the most abundant elements, such as carbon or oxygen (Allende Prieto, Asplund & Lambert 2001, 2002, Asplund et al. 2004, 2005), but minor changes affect also iron (Asplund et al. 2000b), silicon (Asplund 2000), or calcium (Asplund et al. 2005). The latter reference summarizes these revisions, which are based on a new generation of three-dimensional time-dependent (non-magnetic) simulations of the solar surface. Updates have also been made for heavier elements (Sneden & Lawler 2005), albeit their impact on the solar absolute fluxes is only marginal.

In our calculations, we have adopted the mixture proposed by Asplund et al. (2005). Note, however, that this compilation is not based on a homogeneous analysis with a single model atmosphere and a uniform protocol. The abundances for a number of elements are derived afresh, but for others it represents a critical evaluation of new and old results, by different authors with various degrees of simplification, such as a strict adherence to LTE or the adoption of NLTE corrections for some species, which are still unavailable or unreliable for many other, in particular when it comes to 3D calculations.

3.2 Opacities

After the widely-used photoionization cross-sections of Peach (1970), a significant improvement came with the calculations of atomic structure and opacities performed by the international collaboration known as the Opacity Project (Seaton et al. 1992). Until very recently, the Opacity Project (OP) provided
two extreme products: cross-sections for each atomic state, or Rosseland mean opacities. For calculating synthetic fluxes, or model atmospheres, one needs monochromatic opacities, but LTE codes deal most comfortably with opacities per species, and do not need detailed photoionization cross-sections for every single energy configuration. This situation has recently changed with the release of monochromatic opacities for each element as a function of temperature and electron density (Seaton 2005), but the inconvenience of having to deal with cross-sections has likely to do with the slow integration of the OP data in astronomical codes.

We have implemented model atoms and ions for the most relevant species for F-G-K-type atmospheres using the OP photoionization cross-sections (Allende Prieto et al. 2003b). The data format follows the specifications for the NLTE model atmosphere code Thusty (Hubeny & Lanz 1995) and the spectral synthesis code Synspec (Hubeny & Lanz 2000). As the computed energy levels are relatively inaccurate, the location of the predicted resonances (associated with two-electron autoionization; see the review article by Sultana Nahar in this volume) in the cross-sections is uncertain, and therefore we have smoothed them following the prescription proposed by Bautista, Romano & Pradhan (1998). These models continue to be updated periodically, and are publicly available.

The OP calculations cover most elements from hydrogen through calcium, but for iron ions have been superseded by newer results from the Iron Project (see Bautista 1996, 1997, Bautista & Pradhan 1997, Nahar & Pradhan 1996, 1999, and Nahar’s paper in this volume). The distribution of data for Fe I and Fe II (the relevant iron ions for late-type stellar atmospheres) through the Iron Project data base is still patchy, but working in collaboration with Manuel Bautista and Sultana Nahar, I have translated the data files to the same format employed by the OP, and new model atoms for Thusty/Synspec have been produced.

The Iron Project model ions are significantly larger than those for lighter elements based on the OP data, including of the order of 700 energy levels per ion. Assuming the relative populations of levels with similar energies and the same quantum numbers L and S are in equilibrium at a given temperature, it is possible to combine the cross-sections of these levels creating super-levels. The concept of super-levels, introduced by Anderson (1989; see also Hubeny & Lanz 1995), can be exploited to effectively reduce the complexity of the opacity calculations, as well as to speed up the solution of the rate equations in NLTE problems. For a solar-like atmosphere, using this simplification for Fe I (assuming $T = 5000$ K) and for Fe II ($T = 7000$ K), leads to errors in the computed absolute flux less than 1% when the size of the model atoms is reduced tenfold, as shown in Fig. 1.

\[^1\text{http://hebe.as.utexas.edu/at/} \text{and http://nova.astro.umd.edu/}\]
Fig. 1. Ratio of the solar irradiances computed with a simplified and full-blown iron model atoms (Fe and Fe$^+\)). The full-blown models account for the radiative opacity from more than a thousand levels, while the boiled-down models include only about a hundred.

3.3 Equation of state

By adopting a model atmosphere that has been precalculated, all relevant thermodynamical quantities are readily available as a function of the location in the atmosphere. As we discussed above, the input atomic and molecular data, as well as the abundances, will determine the resulting structure and energy flux, but some quantities, such as the emergent flux, are expected to be more sensitive to small variations in some of the basic inputs than others, such as the thermal structure of the model atmosphere.

We have explored the effect of small changes in the input chemical composition on the emergent fluxes by considering the thermal atmospheric structure fixed (see Section 4). Under this approximation, we still recompute consistently the electron density and solve the molecular equilibrium. This step involves a major upgrade from our earlier calculations in order to consider the presence of molecules, their impact on the electron density, and ultimately on the atomic species (I. Hubeny, private communication). To this purpose, the most recent versions of Synspec include routines kindly provided from U. Jörgensen. Both atomic and molecular partition functions are adopted from
Irwin (1981 and private communication), while other molecular data are from Tsuji (1973).

3.4 Model atmospheres

As argued above, computing absolute fluxes involves solving consistently the problem of atmospheric structure and calculating the radiation field for any given set of abundances. We are using a NLTE model atmosphere code, but including in detail all the relevant sources of opacity for late-type atmospheres and accounting for departures from LTE simultaneously is a massive problem. On the other hand, mild or no departures from LTE are expected for many atomic and molecular species. Thus, we are working towards a hybrid scheme where the contribution to the opacity for most species is computed in LTE and stored in a look-up table, while only the most relevant ions are considered in NLTE.

We have already mentioned recent updates in the solar photospheric abundances associated with a new kind of model atmospheres based on 3D hydrodynamics. Surface inhomogeneities, in particular solar granulation, may have an important effect on the absolute flux emerging from the solar surface. Radiative transfer solvers for 3D are typically ready to handle only simple line opacities: one line profile or a few. Computing absolute fluxes, especially in the UV domain, requires including very large number of overlapping atomic and molecular transitions, in addition to detailed metal photoionization cross-sections. To this goal, a new radiative transfer code has been developed by L. Koesterke (private communication), able to consider full-blown opacities, including electron and Rayleigh scattering.

Koesterke et al. (2007) find that the solar 3D model by Asplund et al. (2000a) performs similarly to 1D models regarding limb darkening in the continuum, despite a simplified description of the radiation field. In addition, the same model vastly outperforms 1D models regarding line formation, and in particular the center-to-limb variation of line profiles. The ability of 3D models to match the solar limb darkening had been put into question by Ayres et al. (2006). Based on tests using a horizontal- and time-averaged structure from the simulations by Asplund et al. (2000a), these authors predicted a dramatic failure of the new models. The more rigorous calculations by Koesterke et al. show that the limb-darkening of a three-dimensional model is very different from that of a 1D model derived by taking the average over surfaces with constant vertical optical depth. The effects of surface convection on the absolute solar fluxes are currently being investigated with the new radiative transfer code.
4 The role of chemical composition: a seven-pipe problem

Comparing absolute solar fluxes predicted by model atmospheres with observations usually involves adopting a standard set of chemical abundances, but can we consider the chemical composition as a fixed set of parameters? The recent revisions for carbon and oxygen, together with the typical error bars still quoted in solar abundance studies, which sometimes exceed 0.1 dex, suggest that the answer is NO.

Fig. 2. Relative variations in the solar surface flux emergent from a 1D solar model atmosphere resulting from changes in the adopted chemical composition. The atmospheric structure (the run of temperature versus mass column density) is considered constant in these calculation.

Only a few elements can make an important impact on the computed solar fluxes: directly through contributed opacity, or indirectly, by their effect on the atmospheric structure or the number of free electrons they release through ionization. We have calculated, using a solar Kurucz model, the effect of changing the abundances of the most relevant elements on the solar spectrum. The results of 0.2 dex variations in the X/H ratios, where X is He, C, O, Mg, and Fe, are shown in Fig. 2. Ca, Si, and some iron peak elements can also have an effect.
H$^-$ dominates the continuum opacity in the solar optical and infrared. In the blue and UV, atomic iron and magnesium contribute significant continuum opacity through photoionization, and iron also provides abundant line opacity. At wavelengths shorter than 200 nm, aluminum and silicon need to be considered as well (but see comments in §). Molecules, mainly CH, CO, and OH dominate relatively narrow bands of the optical, IR and UV solar spectrum. Besides H, at least iron, magnesium and silicon, are significant contributors to the pool of free electrons, which has a tremendous impact on the continuum opacity as the number density of free electrons is smaller than that of hydrogen atoms and therefore controls the formation of H$^-$.

At first sight, the impact of changing the helium abundance in Fig. 2 may be a surprise. This is truly an indirect effect: as all abundances are normalized to H and He is very abundant, $N(\text{He})/N(\text{H}) \sim 0.07$, an increase in He/H involves a significant reduction in $N(\text{H})$, and consequently in the atomic hydrogen opacity, which results in an increased irradiance. Fortunately, the solar He/H ratio is known precisely from helioseismology.

Inspection of Fig.2, considering that the observed solar absolute fluxes are likely accurate to a level of $\sim 1\%$ or better, indicates that the current uncertainties in the chemical composition of the solar surface may be a dominant source of error in the flux calculations. This situation is similar to the case of the predicted solar neutrino fluxes! (Bahcall & Serenelli 2005).

5 Conclusions

Observations of the solar angular diameter by different authors and methods still show rather significant discrepancies (see, e.g., Basu 1998, and the references discussed by Wittmann & Neckel 1996), and probably a poorly-understood time variation. Nonetheless, this quantity is known with a relative accuracy many orders of magnitude higher than for any other star, opening the possibility to compare detailed observed absolute fluxes with the predictions from model atmospheres to learn about physics and astronomy.

So far, no assessment has been made of the potential impact of the new generation of the 3D hydrodynamical model atmospheres on the computed solar irradiance, but the presence of inhomogeneities introduced by convective overshooting could alter the solar spectrum significantly. Computing fluxes from 3D models involves 3D radiative transfer; using horizontally-averaged structures to explore 3D models is bound to lead to erroneous conclusions. The availability of several detailed hydrodynamical simulations of the solar surface (e.g., Asplund et al. 2000a, Wedemeyer et al. 2004, Vögler et al. 2005) contrasts with the scarcity of detailed radiative transfer using them.

Computing absolute fluxes is more demanding than relative values, and much more sensitive to input values such as the adopted chemical composition. Modern opacities should be employed, in particular computed state-of-the-art
photoionization cross-sections for atomic iron, magnesium, aluminum, and silicon, as well as line opacity from the most important diatomic molecules. Our tests indicate the need for fully consistent calculations in order to disentangle the impact of changes in composition and input micro-physics. The blue and UV fluxes of the Sun are particularly sensitive to the abundances of hydrogen, carbon, oxygen, magnesium, aluminum, silicon, calcium and iron. Our preliminary results hint that the uncertainties in the composition of the solar atmosphere may be a dominant source of error in predicting the radiation output of the Sun.

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