

Solar oxygen abundance

Maria Bergemann¹,^{1,2} Richard Hoppe,^{1,3} Ekaterina Semenova,¹ Mats Carlsson,^{4,5}
Svetlana A. Yakovleva,⁶ Yaroslav V. Voronov,⁶ Manuel Bautista,⁷ Ahmad Nemer,⁸
Andrey K. Belyaev,⁶ Jorrit Leenaarts,⁹ Lyudmila Mashonkina¹⁰,¹⁰ Ansgar Reiners¹¹
and Monika Ellwarth¹¹

¹Max Planck Institute for Astronomy, D-69117 Heidelberg, Germany

²Niels Bohr International Academy, Niels Bohr Institute, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark

³Ruprecht Karls University, Grabengasse 1, D-69117 Heidelberg, Germany

⁴Rosslund Centre for Solar Physics, University of Oslo, PO Box 1029 Blindern, NO-0315 Oslo, Norway

⁵Institute of Theoretical Astrophysics, University of Oslo, PO Box 1029 Blindern, NO-0315 Oslo, Norway

⁶Department of Theoretical Physics and Astronomy, Herzen University, St. Petersburg 191186, Russia

⁷Department of Physics, Western Michigan University, Kalamazoo, MI 49008, USA

⁸Department of Astrophysical Sciences, Princeton University, Princeton, NJ 08544, USA

⁹Institute for Solar Physics, Department of Astronomy, Stockholm University, AlbaNova University Centre, SE-106 91 Stockholm, Sweden

¹⁰Institute of Astronomy of the Russian Academy of Sciences, Pyatnitskaya st. 48, Moscow 119017, Russia

¹¹Institut für Astrophysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

Accepted 2021 July 7. Received 2021 July 5; in original form 2021 March 5

ABSTRACT

Motivated by the controversy over the surface metallicity of the Sun, we present a re-analysis of the solar photospheric oxygen (O) abundance. New atomic models of O and Ni are used to perform non-local thermodynamic equilibrium (NLTE) calculations with 1D hydrostatic (MARCS) and 3D hydrodynamical (Stagger and Bifrost) models. The Bifrost 3D MHD simulations are used to quantify the influence of the chromosphere. We compare the 3D NLTE line profiles with new high-resolution, $R \approx 700\,000$, spatially resolved spectra of the Sun obtained using the IAG FTS instrument. We find that the O I lines at 777 nm yield the abundance of $\log A(\text{O}) = 8.74 \pm 0.03$ dex, which depends on the choice of the H-impact collisional data and oscillator strengths. The forbidden [O I] line at 630 nm is less model dependent, as it forms nearly in LTE and is only weakly sensitive to convection. However, the oscillator strength for this transition is more uncertain than for the 777 nm lines. Modelled in 3D NLTE with the Ni I blend, the 630 nm line yields an abundance of $\log A(\text{O}) = 8.77 \pm 0.05$ dex. We compare our results with previous estimates in the literature and draw a conclusion on the most likely value of the solar photospheric O abundance, which we estimate at $\log A(\text{O}) = 8.75 \pm 0.03$ dex.

Key words: atomic data – radiative transfer – techniques: spectroscopic – Sun: abundances – Sun: chromosphere – Sun: photosphere.

1 INTRODUCTION

Oxygen is (behind H and He) the most abundant chemical element in the Universe and it is of major relevance in modern astrophysics, across different fields, including precision stellar physics, extragalactic astronomy, planet formation, and galaxy evolution. Most importantly, oxygen determines much of the opacity in the solar interior (e.g. Bahcall, Serenelli & Basu 2005; Pinsonneault & Delahaye 2009; Serenelli et al. 2009), therefore its abundance is critical to the calculation of Standard Solar Models (SSM), which describe the evolution of the Sun from the pre-main-sequence to

the present age of 4.5 Gyr. Oxygen is also the key element in gas-phase spectroscopic diagnostics on extragalactic scales, in particular to infer the metallicities from the H II regions (e.g. Kewley & Ellison 2008; Moustakas et al. 2010) – a broadly used technique that has been applied to many star-forming galaxies to establish their metal-content and to quantify the mass–metallicity relationship across the entire mass range of galaxies in the local universe. Oxygen is also one of the two – in addition to Mg – most common tracers of nucleosynthesis in massive stars, which explode as core-collapse supernovae. Therefore, O abundance is traditionally used in combination with Fe to map the chemical enrichment and star formation history of stellar populations in the Milky Way and its satellite galaxies (e.g. Tolstoy, Hill & Tosi 2009; Barbuy, Chiappini & Gerhard 2018).

This study focuses on the first problem – the chemical abundance of oxygen in the Sun. Over the past decades, several groups approached this problem from various angles. Some groups attempted

* E-mail: bergemann@mpia-hd.mpg.de

† The first two authors have contributed equally to the work presented in this paper.

to measure the O abundances from the solar photospheric spectrum (e.g. Grevesse & Sauval 1998; Allende Prieto, Lambert & Asplund 2001; Asplund et al. 2004; Caffau et al. 2008; Pereira, Asplund & Kiselman 2009b; Sitnova, Mashonkina & Ryabchikova 2013; Caffau et al. 2015; Socas-Navarro 2015; Steffen et al. 2015; Amarsi et al. 2018). Other groups derived the solar O abundances from the high-ionized lines in the solar wind (e.g. Bochsler 2007; Laming et al. 2017). The latter can be, however, measured less accurately compared to the photospheric analysis methods. In the seminal paper, Grevesse & Sauval (1998) presented the O abundance of 8.83 ± 0.06 dex, based on 1D LTE methods. The most recent estimate, derived by means of a detailed NLTE analysis with 3D radiation-hydrodynamic (RHD) simulations of solar convection, is $\log A(\text{O}) = 8.69 \pm 0.03$ dex (Amarsi et al. 2018, based on the 777 nm lines), which compares well within the uncertainties with the estimate by Caffau et al. (2015, based on the forbidden 630 nm line) ($\log A(\text{O}) = 8.73 \pm 0.02 \pm 0.05$ dex). Neither of these estimates, however, are satisfactory for the SSM calculations (Villante & Serenelli 2020), as the internal structure of the present-day solar model – the sound speed profile, the depth of the convective envelope – does not compare well with independent constraints on its structure obtained by means of helioseismology. Various scenarios have been put forward to explain the mismatch, ranging from the underestimated opacity in the interior (Bailey et al. 2015, but see Nagayama et al. 2019) to energy transport by dark matter particles (Vincent, Scott & Serenelli 2015). The problem has, so far, not been convincingly explained by any of these scenarios.

In this work, we present a new spectroscopic analysis of the solar photospheric O abundance. We are motivated by the availability of new atomic data and recent 3D magneto-hydrodynamic (MHD) simulations of near-surface convection, the chromosphere, and the photosphere (Carlsson et al. 2016). Our model atom of O relies on new data describing collisional excitation and charge transfer with H atoms, photoionization, and collisions between O I and free electrons. We also analyse the uncertainty in the oscillator strengths of the transitions observed. In addition, we develop a new model atom of Ni in order to study the influence of the Ni blend in one of the diagnostic O I features. Finally, we investigate the O I line formation using different types of the solar model atmospheres, including the *Stagger* RHD model, but also two 3D MHD models computed self-consistently, with and without chromosphere, using the *Bifrost* code. This is important for any study that requires precision abundance diagnostics, such as, e.g. a detailed analysis of the Sun relative to solar twins, comparative studies of exoplanet hosts, or spectroscopic age indicators (e.g. Bedell et al. 2014; Buchhave & Latham 2015; Bedell et al. 2018; Lorenzo-Oliveira et al. 2018; Nissen et al. 2020).

The paper is organized as follows. Section 2 provides the details of observational data sets used in the abundance calculations. In Section 3 we describe the main properties of the atomic models of O (Section 3.1) and Ni (Section 3.4), in particular, the calculations of new photoionization cross-sections and electron collision rates (Section 3.2), collisions with hydrogen atoms (Section 3.3). In Section 3.5 we review the 1D and 3D (M)RHD model atmospheres, the statistical equilibrium and radiation transfer codes (Section 3.6), and the details of abundance analysis (Section 3.7). We then describe the results of our calculations in Section 4, addressing the following aspects: line formation of O (Section 4.1) and Ni (Section 4.3), centre-to-limb (CLV) variation (Section 4.4), error analysis (Section 4.7), the solar O abundance (Section 4.6). We perform a comparative analysis of our findings in the context of earlier studies in the literature (Section 5). Finally Section 6 summarizes the conclusions and provides an outlook for future work.

2 OBSERVATIONS

In this work, we make use of different spectroscopic data available for the Sun.

Our primary data set are the new spatially resolved solar data obtained with the Fourier Transform Spectrograph mounted on the Vacuum Vertical Telescope at the Institut für Astrophysik Göttingen (hereafter, referred to as IAG data). Light from the 50cm-siderostat is picked up by a fibre with an on-sky diameter of 25 arcsec and sent to the FTS (for more information, see Reiners et al. 2016; Schäfer et al. 2020). The FTS was operated in double-sided mode with a spectral resolution of 0.024 cm^{-1} , i.e. $R = \Delta\lambda/\lambda \approx 700\,000$ at $\lambda = 6\,000 \text{ \AA}$. We collected 123 individual observations of the quiet Sun at 12 different μ -angles during April and August 2020. Each observation took approximately 10 min. We used the HITRAN data base to identify telluric lines from H_2O and O_2 and mask them in the spectra. Relative motion between the VVT and the respective solar position was determined using the ephemeris code (Doerr 2015) based on the NASA’s Navigation and Ancillary Information Facility SPICE toolkit (Acton 1996). We used the differential rotation law of the Sun (Snodgrass & Ulrich 1990) to correct the individual spectra for solar rotation, and we subtracted barycentric and rotational motion from every observed spectrum. Before addition, we normalized individual spectra and corrected remaining radial velocity offsets between different exposures taken at the same μ -angles but at different positions on the Sun. We verified that these offsets were within the range of pointing errors. Eventually, we added spectra observed at the same μ -angles. Our co-added spectra cover the spectral range between 4700 \AA and 7900 \AA and have a signal-to-noise (S/N) of 450 per resolution element at 6000 \AA . In our analysis we employ the μ angles¹: 0.2, 0.4, 0.6, 0.8, 1.0.

We also employ high-resolution spatially resolved spectra (Pereira, Kiselman & Asplund 2009a; Pereira et al. 2009b) obtained with the TRIPPEL (TRI-Port Polarimetric Echelle-Littrow spectrograph) spectrograph mounted on the Swedish 1-m Solar Telescope (hereafter, referred to as SST data) (Scharmer et al. 2003). These data have a resolving power of $R = \lambda/\delta\lambda \approx 200\,000$ and cover the wavelength regions around the O I triplet (7771 to 7775 \AA) and [O I] (6300 \AA) lines.

In addition, we analyse the spatially resolved solar spectra obtained with the Solar Optical Telescope on the *Hinode* satellite (Caffau et al. 2015). These data are not affected by telluric absorption, which is especially critical in the region around 630 nm. The *Hinode* data have a resolving power of $R = 200\,000$ and an S/N of 20 000. The pointings include the following μ angles: 0.38, 0.70, 0.86, 0.95, and 0.99. For a more detailed description of the observations and the data reduction, we refer the reader to Caffau et al. (2015).

We complement the aforementioned data with the very high-quality, $R \approx 350\,000$, disc-centre spectra obtained using the KPNO FTS instrument. These data were released by Brault (1972) and a re-reduced version was published in Neckel & Labs (1984).

The last resource of observational data in this work is the data collected by Takeda & UeNo (2019) using the 60 cm Domeless Solar Telescope (hereafter, referred to as DST data) with the Horizontal Spectrograph at Hida Observatory of Kyoto University. In total, 31 different μ -angles have been observed, of which we were only interested in the disc-centre intensity. The spectra have a resolving power of $R \sim 140\,000$ and S/N of several hundreds.

¹Here $\mu = \cos \theta$ and θ is the heliocentric viewing angle, with the disc centre corresponding to $\theta = 0^\circ$.

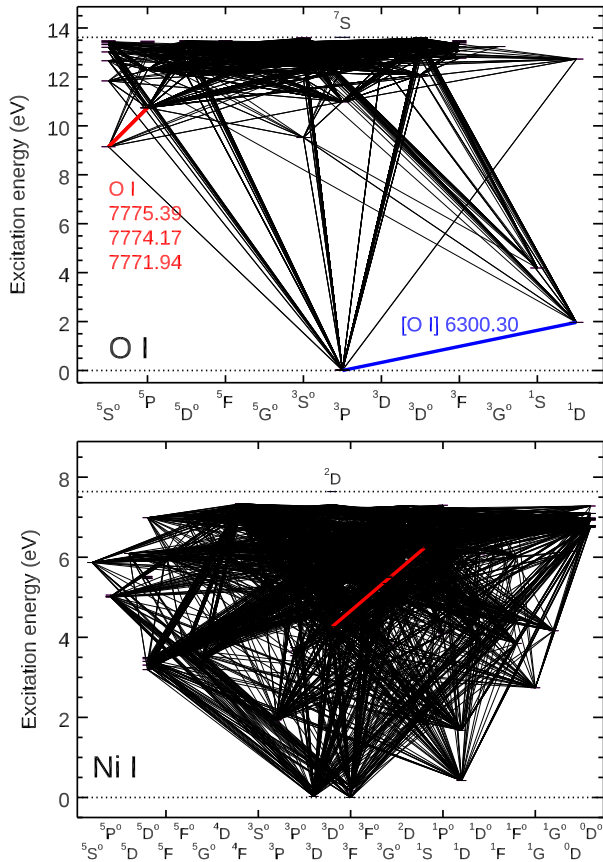


Figure 1. Grotrian models of O (top panel) and Ni (bottom panel). The diagnostic features used in the spectroscopic analysis are indicated using bold blue and red lines.

3 METHODS

3.1 O model atom

The model atom consists of 122 energy states, with neutral oxygen represented by 120 energy states and the singly ionized oxygen by 2 states, the ground state and the first excited state. The energy levels, which includes levels with principal quantum number $n \leq 30$ and orbital angular momentum $l \leq 4$, were assembled from the NIST data base (Kramida et al. 2020). The original number of O I energy levels is 227; however, we merge the fine structure levels with the energy above $102\,700\text{ cm}^{-1}$ (12.73 eV), so that all states above the level $3s^1D^o$ are represented by a term with the statistical weight g obtained by summing the individual statistical weights of the levels and the energy computed by weighted averaging of fine structure level energies according to their g -value (cf. Bergemann et al. 2012). As a result our O I model contains 35 fine structure states and 87 terms. Fig. 1 (top panel) shows the Grotrian diagram of O I, with the key diagnostic transitions in the solar spectrum indicated with bold lines. The majority of lines in the O I system connect energy levels with a very high, $E > 10\text{ eV}$, excitation potential (relative to the ground state).

The diagnostic O lines used in the abundance analysis are the triplet O I lines at 777 nm and the forbidden [O I] line at 630 nm (Table 1). The former lines arise in electric dipole transitions from the $2p^33s^5S_2^o$ level at 9.15 eV above the ground level. The line at 630 nm is a magnetic dipole transition that arises from the ground level $2p^4^3P_2$. This transition is also observed in emission in the

airglow spectra in the terrestrial atmosphere (Rees 1989; Slanger et al. 2011). Owing to its very low transition probability ($\log gf = -9.72$, Storey & Zeippen 2000), the [O I] line is weak even in the solar spectrum and its equivalent width (EW) measures only a few mÅ (see the online Appendix). According to the NIST data base,² the f -values of the 777 nm and the 630 nm transitions have an uncertainty rating ‘A’ (≤ 3 per cent, or better than 0.01 dex) and ‘B+’ (≤ 7 per cent, or better than 0.03 dex), respectively. However, these uncertainty estimates from NIST appear to be highly overoptimistic. The true uncertainties are likely significantly larger, as indicated by the recently published new transition probabilities Civiš et al. (2018) and our own calculations (Section 4.7). In this work, we have chosen to perform all abundance calculations using the average of Hibbert et al. (1991) and Civiš et al. (2018) f -values for the 777 nm lines ($\log gf = 0.343, 0.197, -0.025$ for the 7771, 7774, and 7775 Å lines, respectively), and Storey & Zeippen (2000) data for the 630 nm lines. We furthermore use one half of the difference between Hibbert et al. (1991) and Civiš et al. (2018) (0.026 dex) as a 1σ uncertainty, and adopt a 20 per cent uncertainty (0.08 dex) on the f -value of the magnetic dipole line. We return to this issue in Section 4.7. The parameters of the diagnostic lines of O I are provided in Table 1.

The parameters of all other radiative bound–bound transitions in the O model atom, including wavelength, f -values, damping constants, were taken from the Kurucz³ data base. There are 13 483 radiative transitions in the wavelength range from 666 Å to $100\,000\text{ Å}$. However, after merging the energy states and making a cut on the oscillator strength ($\log gf = -10$), the number of radiative transitions is compressed to 1364. The chosen cut is needed to capture the resolved photoionization and recombination resonances, including the Rydberg Enhanced Recombination (Nemer et al. 2019). These processes lead to a sequence of transitions that involve the diagnostic O I lines, hence they are necessary for the accuracy of the SE calculations. The lines long-ward of $20\,000\text{ Å}$ are important, because they represent a channel through which the majority of very high-excitation states are connected and therefore, ensure their convergence to statistical equilibrium (SE).

Most of the lines in the atomic model are represented by Voigt profiles with nine frequency points, which is sufficient for the SE calculations. The diagnostic O I lines are represented by 251 frequency points. Van der Waals damping, that is, broadening caused by elastic collisions with H atoms, is included using the data from Barklem, Piskunov & O’Mara (2000). It should be noted, though that only 33 of our lines are present in the Barklem et al. (2000) data base, therefore for the remainder of transitions we resort to the standard Unsöld formalism (Unsöld 1955). It is known that the Unsöld theory underestimates line broadening, as it only applies to collisional broadening at large atomic separations. However, this is not of a concern for O I, as our tests with Unsöld damping constants scaled by a factor of 2 and 0.5 yield virtually identical results for the SE and the profiles of diagnostic lines.

3.2 Photoionization and electron collision rates

The standard source of photoionization cross-sections is the Opacity Project (OP) data base TOPbase⁴ (Cunto & Mendoza 1992). However, the data were computed at a very coarse energy resolution

²<https://physics.nist.gov/PhysRefData/ASD/Html/lineshelp.html#OUTAC> C, accessed on and before 2021 May 22. Note the link only works in the copy-and-paste mode in a browser.

³<http://kurucz.harvard.edu/atoms/0800/>

⁴<http://cdsweb.u-strasbg.fr/topbase/topbase.html>

Table 1. Parameters of spectral lines used for the solar O abundance calculation. The wavelengths for the diagnostic lines are taken from the NIST data base. References to the log gf values and H damping are also provided.

Specie	λ [Å]	E_{low} [eV]	E_{up} [eV]	Lower level	Upper level	log gf	vdW	Ref (log gf)	Ref (vdW)
O									
O I	7771.940	9.146	10.741	$3s^5S_2^o$	$3p^5P_3$	0.369, 0.317	453.234	Hibbert et al. (1991), Civiš et al. (2018)	Barklem et al. (2000)
O I	7774.170	9.146	10.741	$3s^5S_2^o$	$3p^5P_2$	0.223, 0.170	453.234	Hibbert et al. (1991), Civiš et al. (2018)	Barklem et al. (2000)
O I	7775.390	9.146	10.740	$3s^5S_2^o$	$3p^5P_1$	0.002, -0.051	453.234	Hibbert et al. (1991), Civiš et al. (2018)	Barklem et al. (2000)
O I	6300.304	0.000	1.967	$2p^4^3P_2$	$2p^4^1D_2$	-9.72		Storey & Zeippen (2000)	Unsöld (1955)
Ni									
Ni I	6300.341	4.266	6.234	$4p^3D_1^o$	$4s^2^1S_0$	-2.11		Johansson et al. (2003)	Unsöld (1955)

assuming the LS coupling and they are available only for the energy states with the principal quantum number of $n \leq 10$. These shortcomings limit the applicability of the OP data to NLTE stellar atmosphere problems.

Also the data that describe the rates of transitions caused by inelastic collisions with free electrons are very sparse. The most recent source of this information is Barklem (2007), who tabulated the rate coefficients for transitions between the seven low-energy states in O I. They employed the standard R-matrix method assuming LS coupling, which is known to deliver relatively accurate results consistent with direct experimental values. These sparse data sets are, however, not sufficient to describe the entire microphysics of interactions between O I atoms, radiation field, and electrons. This is especially important, because the key diagnostic O I lines (the 777 nm triplet) connect very high-excitation energy levels (Fig. 1). Therefore, we opted to compute new photoionization cross-sections and cross-sections for the transitions caused by e–collisions.

We computed new photoionization cross-sections for all levels with a principal quantum number up to $n = 20$ (energies up to $109\,561\text{ cm}^{-1}$). These calculations were carried out with the Breit–Pauli version of the code RMATRIX (Berrington, Eissner & Norrington 1995). This is an implementation of the R-matrix method for atomic scattering calculations. The atomic orbitals for the O^+ target system were obtained with the scaled Thomas–Fermi–Dirac–Amaldi central-field potential as implemented in AUTOSTRUCTURE (Badnell 1997). Our target representation included eleven configurations $2s^23p^3$, $2s^23p^23s$, $2s^23p^23p$, $2s^23p^23d$, $2s3p^4$, $2s3p^33s$, $2s3p^33p$, $2s3p^33d$, $2s^23p3s^2$, $2s^23p3p^2$, and $2s^23p3d^2$. This expansion lets to 26 close coupling LS terms and 39 energy levels with principal quantum number up to $n = 20$.

We give a preference to the new photoionization cross-sections over the TOPbase values. First, our target and close coupling expansions are larger than those of the OP. Second, the present cross-sections are in intermediate coupling and account for relativistic corrections, as opposed to the LS-term OP cross-sections. Finally, we retained level-to-level partial cross-sections, which allow for a reliable determination of recombination rates. Also, our cross-sections have the energy resolution of 2.2×10^{-4} Ryd, (about $100 \times$ better resolution than OP cross-sections), which adequately resolves the cross-section resonances. Fig. 2 compares our new values for two selected energy levels with the TOPbase data. Our cross-sections include more resonance structures, owing to the much larger close-coupling expansion. In the case of the $3s^5S^o$ state, the TOPbase cross-section exhibits an abnormal decreasing trend at higher energies and a sort of bulge at lower energies. Our data show a correct high-energy behaviour and reveal that the bulge is, in fact, a series of resonances, which only show up as proper close-coupling channels are included in the calculations. Regarding the cross-section for the

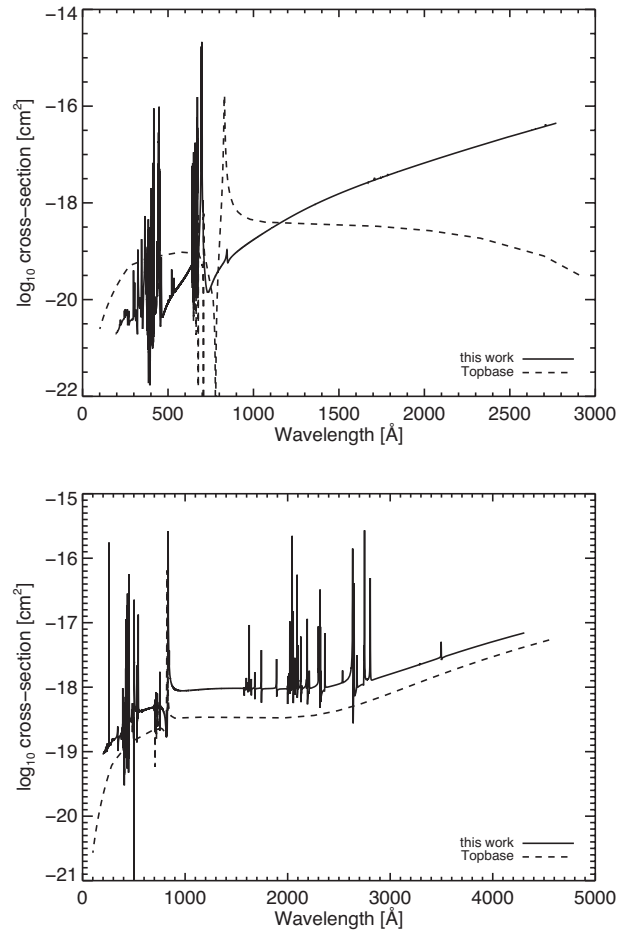


Figure 2. New photoionization cross-sections for the $3s^5S_2^o$ and $3p^5P_1$ levels of O I compared with the Opacity Project data (here we take the cross-section in OP LS-coupling of the 3P for the 5P_1 level).

$3p^5P_1$ level, the results in TOPbase and our data show very similar qualitative behaviour, but our cross-section accounts for more series of resonances. It should be noted that TOPbase only provides data in LS coupling, thus the cross-section shown in Fig. 2 is actually the state’s cross-section.

We also calculated new electron impact excitation rate coefficients using the AUTOSTRUCTURE code (Badnell 2011), which is based on the Breit–Pauli distorted wave method. All configurations of the form $2s^22p^4$, $2s^22p^3nl$, $2s2p^5$, and $2s2p^4nl$, with $n \leq 30$ and $0 \leq l \leq 3$ were included in the calculations. For the rest of the O I system, we complemented the R-matrix collision strengths

with the rate coefficient computed using the formulae from van Regemorter (1962).

3.3 Collisions with hydrogen atoms

Inelastic collisions with H atoms represent an important ingredient in NLTE calculations, as they lead to excitation, de-excitation, ion-pair formation, and mutual neutralization reactions. Detailed quantum-mechanical calculations of the rate coefficients for O were recently presented by two independent groups, Barklem (2018) and Belyaev et al. (2019). These studies rely on different approaches. Barklem (2018) estimated the long-range electronic structure of the OH molecule, by approximating the molecular wavefunction by the linear combination of atomic orbitals (LCAO) of the atoms that form the molecule, while the calculations of collisional dynamics were performed in the framework of the multichannel model (Belyaev 1993), we refer to this approach as LCAO multichannel study. The $O^- + H^+$ scattering channel was not taken into account. Independently, Mitrushchenkov et al. (2019) calculated the electronic structure of the OH molecule using the multireference configuration interaction (MRCI) method and estimated the rate coefficients for $O + H$, $O^+ + H^-$ and $O^- + H^+$ collisional processes using the multichannel model. Later on, Belyaev et al. (2019), based on the MRCI electronic structure by Mitrushchenkov et al. (2019), calculated the rate coefficients for inelastic processes in the same transitions using the quantum hopping probability current (QPC) method. The MRCI QPC study gives a more accurate description of inelastic collisions than the LCAO multichannel study, because it uses a more accurate electronic structure and take into account both the long- and short-range non-adiabatic regions, see Belyaev et al. (2019) for the detailed comparison.

Barklem (2018) tabulate the rate coefficients for the transitions between the lowest 18 terms in OI (up to $3s^1D^o$ at $102\,584\text{ cm}^{-1}$), whereas Belyaev et al. (2019) provide the data for the lowest 11 terms (up to $4s^3S^o$ at $96\,147\text{ cm}^{-1}$). In this work, we complement the latter data with new calculations for five additional states of OI with excitation energies from 12.0786 to 12.5402 eV, as well as two ionic terms $O^+ + H^-$ and $O^- + H^+$. All energy states included in the dynamical calculations are provided in Table 2. For these five additional states the transition probabilities are computed using the asymptotic approach (Belyaev 2013), including the non-adiabatic nuclear dynamical treatment accomplished by the multichannel approach. The calculations are performed within the $4\Sigma^-$ molecular symmetry. Higher-lying covalent states are not included in the calculations, because they either create ionic-covalent avoided crossings at internuclear distances greater than ~ 100 atomic units, and hence the corresponding rates are negligible, or they do not create avoided crossings at all. It should be noted that non-adiabatic transitions between the higher-lying states are possible at short-range distances, although short-range transitions do not lead to high rate coefficients. These rates can be roughly estimated by means of the Kaulakys analytical approach (Kaulakys 1985, 1991). These data sets were recently computed by P. Barklem;⁵ however, only for the lowest 18 energy states of OI that overlap with the states included in the LCAO multichannel calculations. None of the available data sets accounts for the fine structure, therefore, for the lack of a more accurate formulation, we assign the same rate coefficient to each fine structure level within a given term. We note that an alternative approach was proposed in the literature (e.g. Osorio et al. 2015),

⁵<https://github.com/barklem/kaulakys>

Table 2. Scattering channels and the corresponding asymptotic energies, taken from NIST (Kramida et al. 2020).

j	Scattering channels	Asymptotic energies (eV)
1	$O(2p^4\ ^3P) + H(1s)$	0.0000
2	$O(2p^4\ ^1D) + H(1s)$	1.9674
3	$O(2p^4\ ^1S) + H(1s)$	4.1897
4	$O(2p^3\ 3s\ ^5S^o) + H(1s)$	9.1461
5	$O(2p^3\ 3s\ ^3S^o) + H(1s)$	9.5214
6	$O(2p^4\ ^3P) + H(2s)$	10.2000
7	$O(2p^4\ ^3P) + H(2p)$	10.2000
8	$O(2p^3\ 3p\ ^5P) + H(1s)$	10.7406
9	$O(2p^3\ 3p\ ^3P) + H(1s)$	10.9888
10	$O(2p^3\ 4s\ ^5S^o) + H(1s)$	11.8376
11	$O(2p^3\ 4s\ ^3S^o) + H(1s)$	11.9304
12	$O(2p^3\ 3d\ ^5D^o) + H(1s)$	12.0786
13	$O(2p^3\ 3d\ ^3D^o) + H(1s)$	12.0870
14	$O(2p^3\ 4p\ ^5P) + H(1s)$	12.2861
15	$O(2p^3\ 4p\ ^3P) + H(1s)$	12.3589
16	$O(2p^3\ 3s\ ^3D^o) + H(1s)$	12.5402
1	$O^-(2p^5\ ^2P) + H^+$	12.1500
2	$O^+(2p^3\ ^4S^o) + H^-(^1S)$	12.8641

however, also this approach involves an assumption of the relative probability of transitions to different final spin states. Our extensive tests suggest that reducing or increasing the quantum-mechanical rate coefficients by a factor of 3 (which corresponds to the average multiplicity of OI) does not have any significant influence on the SE of oxygen, in line with the findings of Bergemann et al. (2019), thus any further arbitrary manipulation of the data sets is not justified.

Fig. 3 (top panel) shows the data for some the transitions in common between Barklem (2018), our new estimates, and the values estimated using the model of Kaulakys (1985), Kaulakys (1991). Interestingly, there is no systematic difference between the two approaches. For some transitions, Barklem (2018) provide significantly, by up to 4 orders of magnitude, lower rate coefficients. The difference can be explained by the fact that the MRCI QPC study takes non-adiabatic regions at small inter-nuclear distances into account. Due to the transitions at a short range, the probability currents are redistributed differently, as compared to the simplified picture given by including long-range non-adiabatic regions (as done in the LCAO multichannel study) only. This also explain the difference in the rates for the important transitions, $3s^5S^o-3s^3S^o$ and $3s^5S^o-3p^5P$. The rates computed using the Kaulakys (1985, 1991) recipe are typically much larger compared to the data computed using the LCAO multichannel or the MRCI QPC studies. The differences are most significant for transitions with $\Delta E \gtrsim 2.5$ eV. In this regime, the Kaulakys model predicts the rate coefficients that are up to 10 orders of magnitude higher compared to the detailed quantum-mechanical calculations. This is not surprising, as the model was developed to describe transitions between high-energy Rydberg states.

Fig. 3 (bottom panel) illustrates the rate coefficients of ion-pair formation processes computed using the MRCI QPC and the LCAO multichannel methods. There is no significant difference for the majority of the ion-pair formation processes, except the processes with $\Delta E < -2.5$ eV. But the general behaviour of all ion-pair formation processes is very similar.

It is worth pointing out that the scattering channels $j=9-13$ belong to the so-called ‘optimal window’, in accordance with the general behaviour found by applying the simplified model (Belyaev &

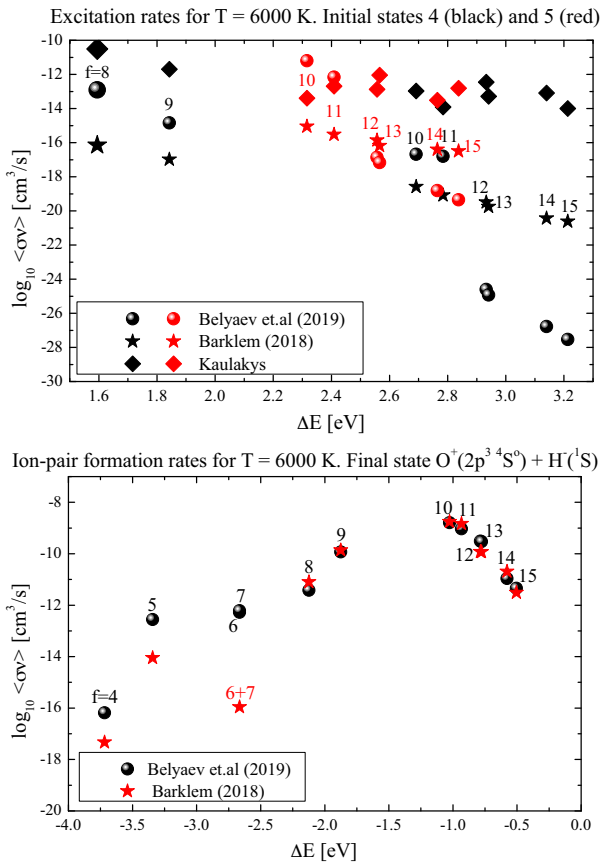


Figure 3. Rate coefficients of the excitation ($\Delta E > 0$) and ion-pair formation processes in $O + H$ collisions at $T = 6000$ K as a function of the energy defect ΔE for the initial (top panel) and final (bottom panel) channels $i = 4$ and $i = 5$ (Table 2). Three sets of data, Barklem (2018), Belyaev et al. (2019), and Kaulakys (1991), are shown.

Yakovleva 2017). The model predicts the largest rates for mutual neutralization processes with final-state binding energies in the vicinity of -2 eV, that corresponds to the excitation energy of 11.65 eV for the OH molecule. This optimal window is well understood through the simplified model and it describes the mechanisms of inelastic atomic collision processes due to long-range non-adiabatic regions created by the ionic-covalent interaction.

Since the LCAO multichannel, MRCI QPC, and Kaulakys data represent physically different approaches to the determination of H impact transition rates, we proceed as follows. We create three NLTE atomic models of O and use them independently in the statistical equilibrium and radiative transfer calculations. One of the models includes the LCAO multichannel data only (hereafter, the LCAO model atom). The other model relies on the LCAO multichannel data co-added with Kaulakys rate coefficients (hereafter, the LCAO+Kaul model), which is appropriate because the LCAO multichannel data describe long-range interactions only and the Kaulakys data are expected to compensate for the lack of short-range interactions. The third model (hereafter, the QPC model) relies on the new rates computed using the MRCI molecular structure and the hopping probability current method. Since in all atomic models, less than 20 energy states (out of 120 O I states in the model atom) are represented with detailed quantum-mechanical data, we connect all other energy states by collision-induced transitions with the rate coefficients computed using the scaled Drawin’s formula (Drawin

1968). As we show in Section 4.2, the only effect of this approach is that it ensures the collisional coupling with the entire O I system and, therefore, helps to greatly speed up the convergence in the very time-consuming 3D NLTE calculations. Both atomic models also include the rates of charge transfer between the O^+ and H^- ions, computed self-consistently using the methods discussed above.

3.4 Ni model atom

Since one of the critical diagnostic O I lines is blended by Ni, we have opted for performing a detailed study of NLTE effects in Ni. To the best of our knowledge, this is the first analysis of the statistical equilibrium of Ni with a comprehensive atomic model with 1D and 3D model atmospheres.

Similar to O, the atomic data for Ni I and Ni II were adopted from the Kurucz data base.⁶ The initial data sets comprise 281 energy levels and 9663 radiative transitions for Ni I, and 716 energy levels and 56 193 radiative transitions for Ni II, respectively. The Ni I levels are taken from the Litzèn, Brault & Thorne (1993) study, which combines experimental measurements with theoretical calculations of the energy level structure. We merge fine structure levels below 6.237 eV and remove transitions with $\log gf < -10$. The uppermost Ni I level in our model has the energy of 7.34 eV, whereas the first ionization threshold (ground state of Ni II) is located at 7.64 eV. We note that there are only two known energy levels of Ni I that are higher than our threshold for Ni I and are below the 1st ionization threshold. One of them has the energy of 7.43 eV ($59940.517 \text{ cm}^{-1}$) and it represents one of the fine structure levels of the $3d8(3F)4s(4F)5p^5D^o$ term. This level is, therefore, merged with the other lower-energy FS levels of this term. The other level is the $3d8(3F)4s(4F)6s^5F$ state with the energy of 7.43 eV ($59862.611 \text{ cm}^{-1}$). Owing to its small J-value ($J = 5$) and a very small number of lines connecting it with the rest of Ni I, we merge it with the Ni I state at 7.34 eV. We have verified that our NLTE results do not depend on the treatment of these 2 levels. Our final model of Ni comprises 538 energy states and 2468 spectral lines represented by Voigt profiles with a nine point frequency quadrature. The first ionization threshold of Ni I is located at 7.64 eV and that of Ni II at 18.17 eV. The Grotrian diagram of Ni I is shown in Fig. 1 (bottom panel). Ni has a very complex energy level system with many singlet, triplet, and quintet terms. It should be noted that this diagram only shows energy levels with an LS designation and it is not complete, as many energy levels in Ni I are described in $J_c K$ coupling scheme (Litzèn et al. 1993).

Our model atom does not include isotopic splitting and hyperfine structure (for the odd Ni components), as the shifts are very small. Using the data from Johansson et al. (2003), we find, for example, that including the two main isotopes of Ni changes the equivalent width of the Ni I line at 6300.342 \AA by less than 0.5 per cent. Therefore, we neglect isotopic shift in the SE calculations of Ni and in the abundance analysis of O.

The photoionization cross-sections were computed using the hydrogenic approximation. The rates of collisional excitation by electrons and hydrogen atoms were calculated using the standard formulae of van Regemorter (1962) and Drawin (1968). We apply a scaling factor of 0.05 to the rates that describe the collisions of Ni I atoms with H, because the standard formulae are known to severely overestimate the rate coefficients compared to the detailed quantum-mechanical data (Barklem 2016). However, we investigate

⁶Taken from <http://kurucz.harvard.edu/atoms/2800/>, using the files alitzen2800.dat, b2800e.com, and b2800o.com

in Section 4 how this assumption influences the results. The rates of collisional ionization were computed using the Seaton (1962) formula.

3.5 Model atmospheres

We use several types of the solar model atmospheres computed under different physical assumptions. The main difference between the types of models is the treatment of geometry and convective energy transport, as described in the subsequent sections.

For the purposes of comparison with previous calculations in the literature (Asplund et al. 2004; Amarsi et al. 2018), we employ the solar MARCS model also used in Bergemann et al. (2019). This is a 1D LTE line-blanketed model atmosphere computed under the assumption of hydrostatic equilibrium. Convective energy transport is parametrized using the mixing-length-theory (MLT), with the MLT α constant set to 0.5. The microturbulence parameter is set to 1 km s^{-1} .

The 3D model atmospheres employed in this paper were computed using two 3D RHD codes. The STAGGER code (Nordlund & Galsgaard 1995; Nordlund, Stein & Asplund 2009) provides a well-established 3D RHD simulation of subsurface stellar convection. The solar simulation used in this work (Collet, Magic & Asplund 2011; Magic et al. 2013) encompasses the entire photosphere as well as the upper part of the convective zone. Bifrost is a 3D (M)RHD code capable of simulating the magnetic solar chromosphere (Gudiksen et al. 2011). We used a Bifrost simulation ranging from ≈ -2.5 Mm below the optical surface up to 8 Mm above. From one snapshot of this full-fledged ‘chromospheric’ simulation, we extracted a purely ‘photospheric’ simulation by cutting off the layers above 1 Mm height. This simulation was given 15 min to re-adjust to the new boundary. The horizontal extent of the STAGGER atmosphere is 8×8 Mm, whereas it is 12×12 Mm for the Bifrost atmosphere. Yet both are large enough to host at least 10 granules at the surface, and have the (x, y, z) -resolutions of $240 \times 240 \times 230$ (STAGGER) and $512 \times 512 \times 512$ (Bifrost), respectively. The horizontal resolution of all models was scaled down to allow for repeated NLTE calculations with modest computational cost. Our detailed tests (Fig. 13, also see Section 4.7) allow us to conclude that (x,y) resolutions in excess of (30,30) are not necessary, as already this configuration preserves the main physical properties of line formation and yields line profiles that differ by no more than 2 per cent from the full geometric set-up. This uncertainty is subdominant to other sources of error in the abundance analysis and can be tolerated. Nonetheless, we account for this error in the determination of the solar O abundance (Section 4.6). The vertical resolution remains unaffected, namely 230 grid-points for the STAGGER simulation and 512 or 192 grid-points for the chromospheric and photospheric Bifrost simulations, respectively.

STAGGER and Bifrost codes differ in the input abundances and in the equation of states (EOS). STAGGER is using a modified version of the EOS from Mihalas, Dappen & Hummer (1988) and abundances from Asplund et al. (2009). The Bifrost simulation used here was originally made to make comparisons with older simulations from Stein & Nordlund and used an EOS from Gustafsson (1973), abundances and continuum opacities from Gustafsson et al. (1975) computed using the Uppsala background opacity package (Gustafsson 1973).

The temperature structure of the combined down-scaled snapshots of all models is shown in Fig. 4. The dashed lines present the structure of the spatially and temporally averaged ((3D)) model atmospheres. The averaged models were computed by interpolating the full 3D

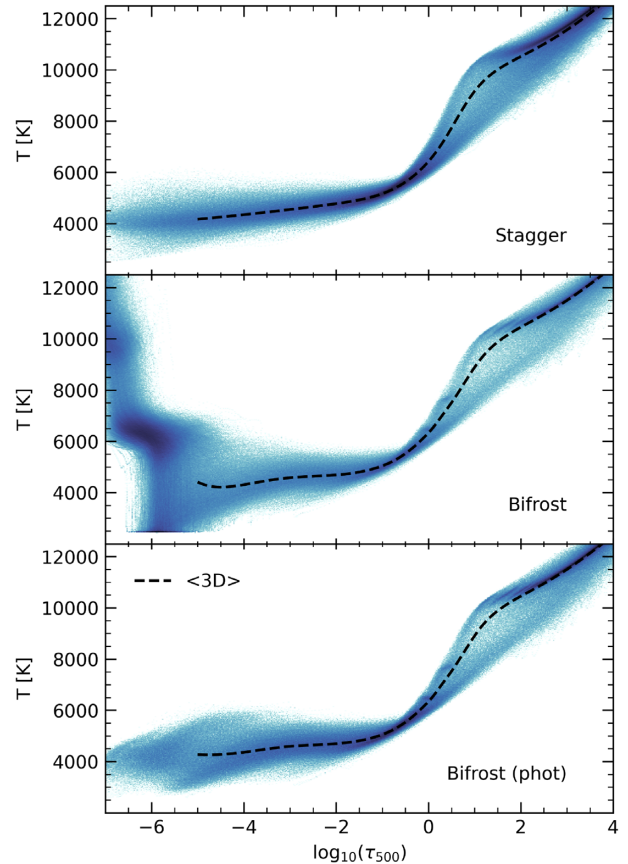


Figure 4. Temperature structure of the STAGGER and Bifrost 3D (M)RHD models as a function of logarithmic optical depth at 500 nm $\log \tau_{500}$. The dashed lines show the $T(\tau)$ structure of the corresponding (3D) averages. See the text.

cubes to an equally spaced optical depth scale and averaging over horizontal slices of equal optical depth. Subsequently all variables were averaged temporally over all spatially averaged snapshots. This was done directly for the temperature and velocity field, but in the case of electron density temporal and horizontal averaging was performed on logarithm of electron number density. The temperature and vertical velocity distributions of the representative STAGGER and Bifrost model atmosphere snapshots are shown in Fig. 5.

3.6 NLTE statistical equilibrium calculations in 1D and 3D

We use two SE codes, MULTI2.3 (Carlsson 1992) and MULTI3D (Leenaarts & Carlsson 2009; Leenaarts, Carlsson & Rouppe van der Voort 2012), both updated as described in Bergemann et al. (2019) and Gallagher et al. (2020). MULTI2.3 solves the detailed equations of SE in a 1D plane-parallel geometry using the Accelerated Lambda Iteration (ALI) method (Rybicki & Hummer 1991, 1992). Radiation transfer is solved by the method of long characteristics. All calculations in this work were carried out using the local operator acting on the source function. MULTI3D solves the radiative transfer equations in 3D geometry on a Cartesian mesh via the short characteristics method (Kunasz & Auer 1988). It is also capable of solving radiative transfer column-by-column mode, that is ignoring the influence of slanted rays. Extensive tests of the full 3D and the column-by-column solution revealed that the differences between the both approaches are negligibly small, especially for the Sun, as the line EWs change by less than 0.5 per cent (see, e.g. the tests carried out by Bergemann

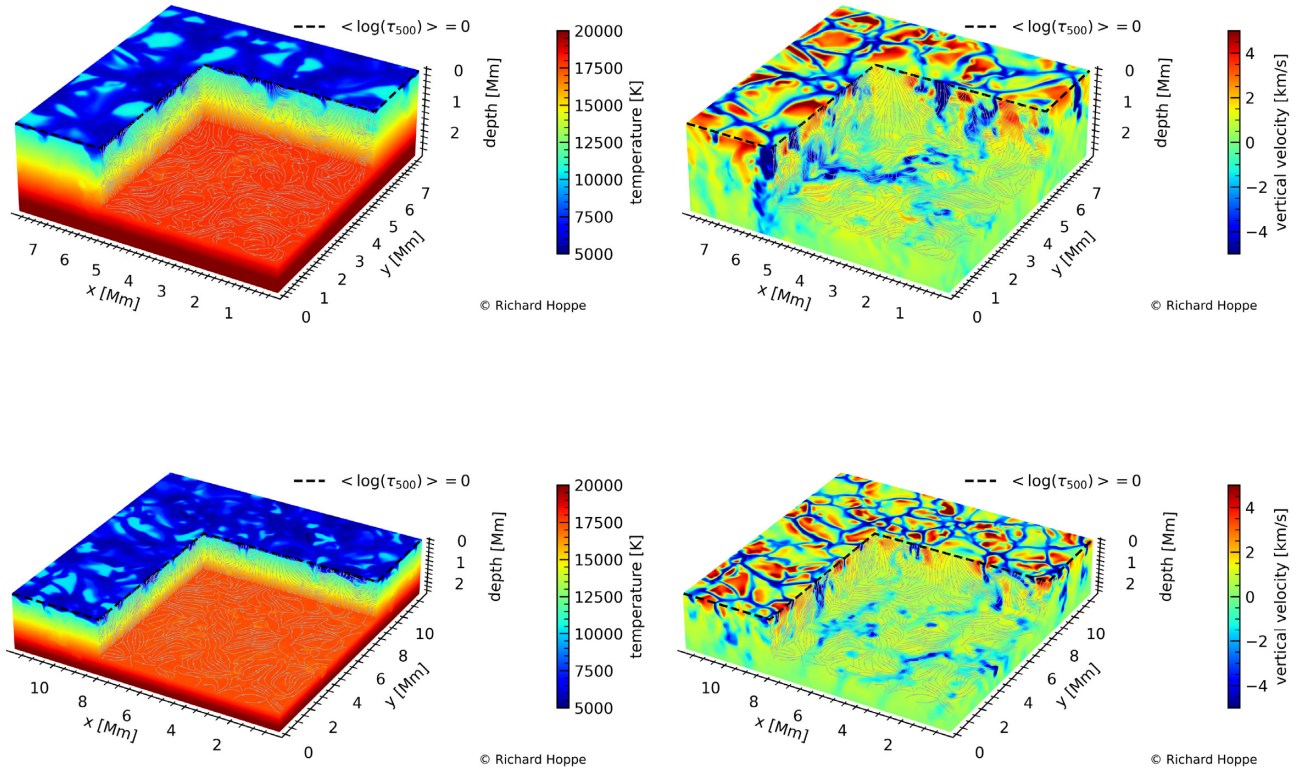


Figure 5. Temperature and vertical velocity distributions of a representative Stagger (top) and Bifrost (bottom) model atmosphere snapshots. Both models have the full horizontal resolution, but, for illustration, we do not show the part of the atmosphere above $\log \tau_{500} \approx 0$. The location of the horizontally averaged optical depth surface is indicated with a dashed line.

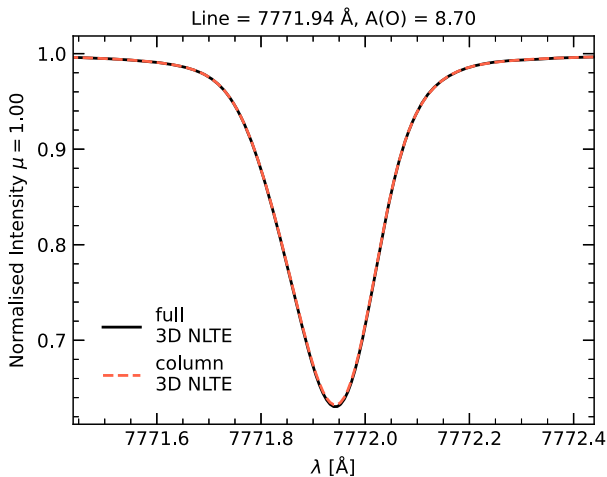


Figure 6. Line profiles of the O I 7771.94 Å line calculated using the column-by-column 3D NLTE solver and the full 3D NLTE radiative transfer solver. The difference in the line EW is only 0.6 per cent.

et al. 2019). Our calculation for the O lines also shows that the difference is only 0.6 per cent (Fig. 6). Therefore, we employ the column-by-column radiative transfer solution with MULTI3D in this work.

In addition to continuum opacities, both MULTI2.3 and MULTI3D are capable of including background line opacity in the form of a linelist. For O, this not important, because the statistical equilibrium of the element is not sensitive to line blanketing. For Ni I, however, a comprehensive treatment of line blanketing across the entire UV

and optical wavelength ranges is critical, because the element, similar to other Fe-group species, is photoionization-dominated. Since MULTI2.3 is also capable of including sampled opacities, we use the code to compute 3D NLTE corrections for Ni separately using the column-by-column solver and apply them to 3D LTE calculations for Ni, in order to get 3D NLTE line profiles of Ni I lines. This approach is needed, because it is currently not feasible to run MULTI3D with a linelist that is comprehensive and detailed enough, that is, which includes the bound-bound transitions of all relevant absorbers across the entire range of frequencies in the Ni model atom. We have verified (see also Gallagher et al. 2020), that both codes provide identical results when the same initial conditions are used. A detailed analysis of the influence of line blanketing in 3D NLTE calculations for different chemical elements will be presented elsewhere.

3.7 Abundance calculations for O and Ni

The calculations of O abundance were carried out using the model atmospheres described in Section 3.5. In the 3D analysis, we employ 13 consecutive STAGGER snapshots, as well as 10 consecutive snapshots for each of the two Bifrost model atmospheres (with and without chromosphere). All model atmospheres were probed by 17 rays at 5 different angles, one ray being the disc-centre intensity ($\cos \theta = \mu = 1$) and the other 16 rays going north, east, south and west at inclinations $\mu = 0.8, 0.6, 0.4,$ and 0.2 in order to match the IAG and SST observations.

We use this set-up to compute O I line profiles for a dense grid of O abundances, sampling the $\log A(O)$ range from 8.50 to 8.90 dex in 3D and 8.50 to 9.20 dex in 1D. Since the diagnostic lines of O

are not strong, it is sufficient to assume an equidistant abundance spacing of 0.2 dex. For Ni, we assume the meteoritic abundance of $\log A(\text{Ni}) = 6.23$ dex from Lodders (2003). This quantity has an uncertainty of 0.04 dex, and it appears to be superior to the values inferred by spectroscopic methods. Asplund et al. (2009) find the Ni abundance of 6.22 ± 0.04 dex, using 3D LTE modelling. This value is significantly higher than the 3D LTE value recommended by Caffau et al. (2015) ($\log A(\text{Ni}) = 6.11 \pm 0.04$ dex). The 1D LTE estimate by Wood et al. (2014), based on the analysis of 76 Ni I and Ni II lines, is 6.27 ± 0.06 dex. We adopt the meteoritic Ni abundance in our work, because of the aforementioned differences in the photospheric results by different groups. We return to this issue in Section 5.

The region around the forbidden [O I] line is modelled by co-adding the profiles of the O and Ni lines in 1D LTE, 1D NLTE, or 3D NLTE respectively and fitting the combined line profiles to the observations. Comparing this approximate approach to the exact procedure, in which the absorption coefficients are co-added instead of the intensity or flux profiles, we find that it provides an almost identical solution (differing in EW by less than 0.5 per cent). Our detailed approach to the model-data comparison and abundance diagnostics is described in Sections 4.4 and 4.6.

4 RESULTS

In this section, we describe the results of our calculations using different model atmospheres and model atoms. We start with a brief overview of the formation properties of O I lines in Section 4.1, continue with the statistical equilibrium of Ni in Section 4.3, discuss our results for the spatially resolved spectra in Section 4.4 and for different atomic models in Section 4.5, and comment on the relevance of 3D (M)HD in the abundance calculations in Section 4.7.3. We then summarize the methods used in the probabilistic abundance analysis and present the final O abundances in Section 4.6. Finally, we compare our results with recent estimates in the literature in Section 5 and draw conclusions.

4.1 O line formation

The formation of O triplet lines at 7771, 7774, and 7775 Å has been a subject of intense discussions over the past decades. Kiselman (1991) was among the first to point out that for the solar model atmosphere the NLTE effects in the diagnostic O lines, which connect the two high-excitation states, are relatively insensitive to the detailed structure of the model atom and are controlled by scattering in the lines. The formation of O triplet lines in the solar photosphere was extensively discussed in Asplund et al. (2004), Steffen et al. (2015), and Amarsi et al. (2018).

Our calculations confirm that the NLTE effects in the triplet lines are mostly driven by photon losses in the lines (Bergemann & Nordlander 2014) that leads to the deviation of the line source function from the Planck function. The overpopulation of the lower level comes at the expense of the ground state population of O I, via a sequence of transitions that involve charge exchange reactions with O II, re-combinations to the high-excitation O I levels, and spontaneous transitions to the lower levels. This is illustrated in Fig. 7, which shows the departure coefficients b_i of the lower $3s^5S_2^o$ and upper $3p^5P_3$ energy states, which connect the diagnostic triplet lines, against the continuum optical depth at 5000 Å. Owing to the small Boltzmann factor, the line formation is restricted to a very narrow range of optical depths ($-1 < \log(\tau_{500}) < 0$). In this region, the ratio of the departure coefficients of the upper and lower energy states drops below unity, $b_j/b_i < 1$. As a consequence, the NLTE

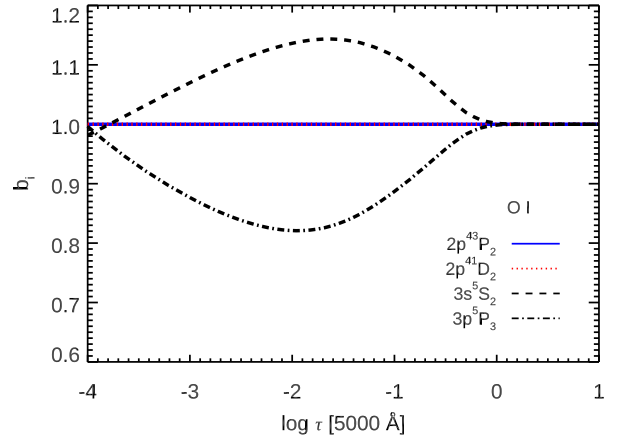


Figure 7. Departure coefficients of the energy levels involved in the diagnostic transitions of O I.

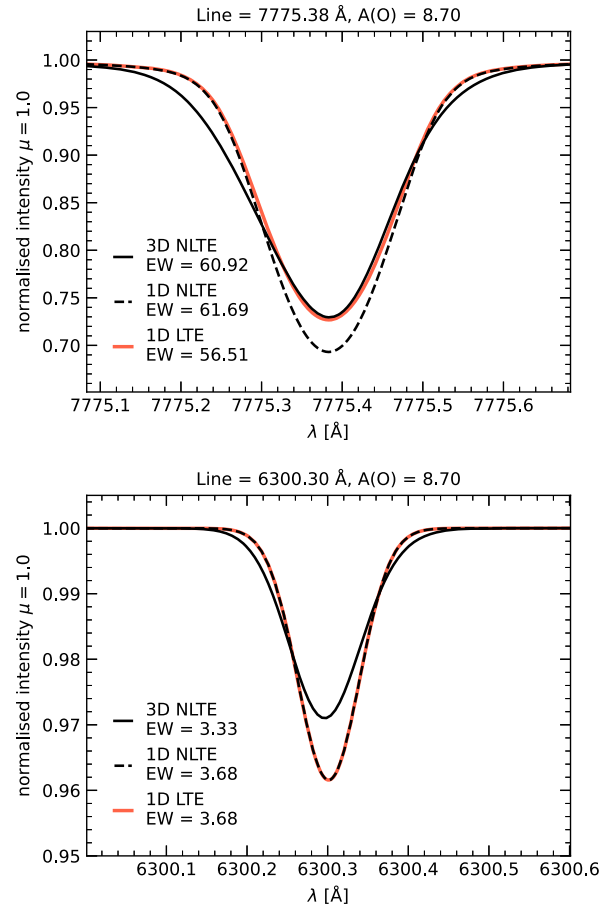


Figure 8. Model 1D LTE, 1D NLTE, and 3D NLTE line profiles of the O I lines at 7775.39 Å (top panel) and 6300.3 Å (bottom panel).

profiles of the permitted O I lines at 777 nm come out stronger compared to the LTE line profiles (Fig. 8, top panel). In contrast, the departure coefficients of the levels involved in the transition (the [O I] line at 630 nm) are very close to unity and the NLTE effects in the line profiles are negligibly small (Fig. 8, bottom panel).

This formation of permitted O I lines is very similar in 1D NLTE and in 3D NLTE (see also Asplund et al. 2004; Steffen et al. 2015; Amarsi et al. 2018). The 777 nm lines are stronger in 3D NLTE

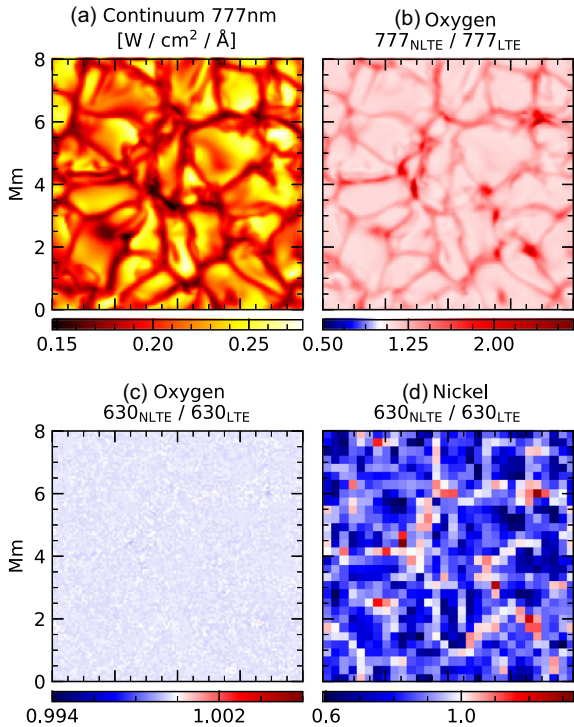


Figure 9. Model continuum intensity in the region of 777 nm is shown in panel (a) in absolute units of $W \text{ cm}^{-2} \text{ \AA}^{-1}$. Ratios of NLTE to LTE EWs of the oxygen 777 nm triplet lines (panel b), oxygen 630 nm line (panel c), and nickel 630 nm line (panel d) computed using the Stagger model atmosphere.

compared to 1D LTE or 3D LTE, that is, the abundances inferred from 3D NLTE line profiles are significantly lower. The forbidden line is barely sensitive to NLTE effects, even in 3D convective models. This is demonstrated in Fig. 9, which shows the absolute continuum intensities (panel a) and the ratios of the NLTE and LTE equivalent widths computed using the Stagger 3D model atmosphere for the 777 nm triplet (panel b) and for the [O I] line at 6300 Å (panel c). The 777 nm lines are stronger in 3D NLTE compared to 3D LTE across the entire simulation surface and the NLTE effects are particularly prominent for the lines that form above the inter-granular lanes. The forbidden [O I] line forms nearly in LTE, although very weak departures from LTE (line weakening in NLTE) are present above the inter-granular lanes.

4.2 O NLTE abundance corrections

Table 3 compares the results in terms of 1D NLTE and 3D NLTE abundance corrections, that is the amount by which the abundance of O has been changed in order to match the EWs of 1D NLTE and 3D NLTE line profiles to those of 1D LTE line profiles. These quantities were computed for the disc-centre intensity and fluxes using the O abundance of 8.70 dex.⁷ The abundance corrections are not used in the abundance analysis, but are useful for their didactic value.

Not surprisingly, the NLTE results and, consequently, the NLTE abundance corrections depend strongly on the input atomic data, foremost on the rates of H impact transitions. Using the quantum-mechanical data (LCAO or QPC), we obtain the 1D NLTE corrections

in the range from -0.20 dex (7771 Å line) to -0.16 dex (7775 Å line) for the LCAO model, and -0.17 dex (7771 Å line) to -0.14 dex (7775 Å line) for the QPC model. However, the results change dramatically, if we include the Kaulakys data in the model, by co-adding them with the LCAO data sets. In this case, the 1D NLTE corrections do not exceed -0.11 dex for the 7771 line and -0.08 dex for the 7775 Å line. All other quantities in the atomic models, such as the representation of H-impact transition rates for the high-excitation energy states, electron collisions, or photoionization, do not influence the results at any significant level. Likewise, the NLTE level populations and the profiles of the diagnostic lines remain nearly identical, regardless of whether Drawin's rates or a blanket constant rate coefficient of 10^{-20} are assumed for the majority of the uppermost states in O I (online Fig. A1 in the online Appendix). As emphasized, however, it is important to include these values to ensure rapid convergence, which is important especially in extremely time-consuming 3D NLTE calculations.

The NLTE corrections computed using the spatially and temporarily averaged (3D) Stagger model atmosphere are less extreme. For the LCAO and QPC atomic models (no Kaulakys data), the largest (3D) NLTE corrections do not exceed -0.16 dex and -0.13 dex (the 7771 Å line), respectively. The model atom that includes LCAO and Kaulakys data returns the results that are not too different from LTE: the largest NLTE correction amounts to -0.06 dex (7771 Å line), whereas the 7775 Å line forms nearly in LTE, with the NLTE correction of only -0.02 dex.

Interestingly, the 3D NLTE abundance corrections are very close to the (3D) NLTE results, although the former are slightly larger in absolute value. For the LCAO model atom, the 3D NLTE corrections amount to -0.17 dex for the 7771 Å line, -0.15 dex for the 7774 Å line, and -0.14 dex for the 7775 Å line. The latter line, which is the weakest of all three, is most sensitive to the structure of the model atmospheres and to the properties of the model atom. Its NLTE correction changes from -0.16 to -0.02 , depending on the details of modelling. The forbidden oxygen line forms almost in LTE, but it shows a non-negligible sensitivity to convection. The 3D NLTE correction for the 630 nm [O I] line amounts to $+0.05$ dex relative to 1D LTE.

Table 3 also shows our 1D NLTE and 3D NLTE corrections for fluxes computed using the LCAO model atom. These results can be directly compared to the corresponding values from Asplund et al. (2004, their table 2). In 1D NLTE, they obtain -0.24 dex for the 7771 Å line, -0.23 dex for the 7774 Å line, and -0.20 dex for the 7775 Å line. In 3D NLTE, they derive -0.27 dex for the 7771 Å line, -0.24 dex for the 7774 Å line, and -0.20 dex for the 7775 Å line. Our values are in a good agreement with this study, although the amplitude of our NLTE corrections is slightly larger. This can be explained by the complexity of the atomic model. Our model includes 120 states of O I coupled by a variety of processes (Section 3.1, whereas the atomic model employed by Asplund et al. (2004) includes only 20 O I states coupled by 43 radiative b-b transitions and electron collisions, and it neglects H-impact collisions. Since the model atom from that study was not published, to check the influence of model atom completeness we performed a sequence of calculations in 1D NLTE (using the MARCS and (3D) model atmosphere), progressively reducing the complexity of the model atom down to 22 levels coupled by 57 radiative b-b transitions. We find that the model that includes 41 oxygen states, with O I closed by the $4f^3F$ term ($102\,968 \text{ cm}^{-1}$) reproduces exactly the results obtained using the complete model. However, atomic models smaller than this limit lead to more modest NLTE corrections. A 22-level atom underestimates the NLTE corrections by 0.07 dex,

⁷We note that the correction is almost identical, if the abundance of 8.90 dex is adopted.

Table 3. 1D NLTE and 3D NLTE abundance corrections for the disc-centre ($\mu = 1$) intensities and fluxes of the diagnostic lines of O. The model atoms are defined as follows (Section 3.1): (a) LCAO data, (b) QPC data, and (c) LCAO data supplemented with the Kaulakys data.

Line (Å)	Intensity ($\mu = 1$)						Flux					
	1D NLTE			(3D) NLTE			3D NLTE			LCAO		
	a	b	c	a	b	c	a	b	c	1D NLTE	(3D) NLTE	3D NLTE
7771.940	-0.20	-0.17	-0.11	-0.16	-0.13	-0.06	-0.17	-0.15	-0.08	-0.28	-0.27	-0.31
7774.170	-0.18	-0.16	-0.10	-0.14	-0.11	-0.05	-0.15	-0.13	-0.07	-0.26	-0.24	-0.29
7775.390	-0.16	-0.14	-0.08	-0.11	-0.08	-0.02	-0.14	-0.12	-0.07	-0.23	-0.20	-0.27
6300.304	0.00	0.00	0.00	+0.04	+0.04	+0.04	+0.05	+0.05	+0.05	0.00	+0.04	+0.04

resulting into 1D NLTE corrections of the order -0.21 (7771) to -0.16 dex. The residual differences can be explained by Asplund et al. (2004) not including H-impact collisions in their model and using the older version of the Stagger model (Asplund, private communication).

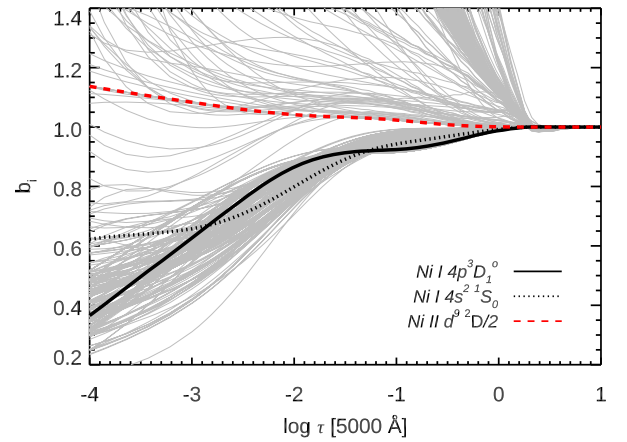
In summary, our findings are similar to those of the previous studies of 1D NLTE and 3D NLTE line formation of O I lines in the solar atmosphere. As we will show below, however, the details of the O I model atom (primarily, the H collision data) and the approach to the statistical analysis of spectral lines, lead to quantitatively different results, when it comes to the analysis of the solar photospheric O abundance.

4.3 Ni line formation

The statistical equilibrium of Ni was previously investigated by Bruls (1993). Using a model atom with 19 energy levels and 81 radiative transitions, they found that Ni I is subject to overionization and line pumping, the processes that generally favour underpopulation of energy levels and cause weakening of spectral lines compared to LTE. Overionization and pumping are driven by strong non-local UV radiation field and, similar to other Fe-group species (Bergemann et al. 2012), influence the levels with excitation energies of ~ 3 to 4 eV. Ding, Qiu & Wang (2002) used a simplified 10-level version of the model developed by Bruls (1993) in order to study the NLTE line formation properties of the at 6767.8 Å line, which is typically used in helioseismology. Vieytes & Fontenla (2013) developed a larger model atom, including 61 energy levels and 401 radiative transitions, and applied the model atom in the calculations of the solar broadband spectrum. None of these studies considered the formation of the Ni I feature at 6300.341 Å that contaminates the [O I] line.

Our calculations confirm that Ni I behaves as a classical minority element with numerous important ionization edges in the UV, which is subject to overionization by strong non-local radiation field. As seen in the diagram of the departure coefficients (Fig. 10), the majority of energy levels in Ni I are underpopulated. The states with excitation energies of 2–4 eV are overionized, whereas the higher-lying Ni I states are collisionally coupled with the latter and therefore display similar NLTE effects. The ground state of Ni II is nearly thermalized across the entire optical depth scale, but higher-lying Ni II states are overpopulated, closely resembling the behaviour seen in other Fe-group elements, such as Cr, Ti, Mn, and Co.

Table 4 presents the 3D LTE, 1D NLTE, and 3D NLTE corrections for the key Ni line at 6300.34 Å. The line is clearly sensitive to convection, with the 3D LTE estimate being higher by 0.06 dex compared to 1D LTE. The NLTE values were computed using three atomic models of Ni, which differ only in the scaling factor to Drawin's ionization rates. For the excitation rates, we used the scaling factor of 0.05 (Section 3.4). Clearly, assuming no H-impact ionising collisions ($S_{\text{bf}} = 0$) or increasing them by a factor of 100 ($S_{\text{bf}} = 100$)

**Figure 10.** NLTE departure coefficients of energy levels in Ni I. The levels involved in the 6300.341 Å transition are highlighted.**Table 4.** 1D and 3D NLTE abundance corrections (in dex) for the disc-centre intensities of the Ni I line at 6300.341 Å. S_{bf} is the scaling factor to the collisional ionization rates computed using the Drawin formula.

Line	LTE		NLTE				
	3D	0	1D	1000	0	100	1000
6300.341	0.06	0.15	0.08	0.02	0.21	0.14	0.08

has a significant influence on the NLTE correction, which changes from $+0.15$ dex to $+0.08$ dex (MARCS) and from $+0.21$ dex to $+0.14$ dex (3D Stagger) respectively. Assuming very large – likely unrealistically too large – Drawin's collisional rates ($S_{\text{bf}} = 1000$), the difference between 3D NLTE and 3D LTE effectively vanishes. The scaling factors of $S_{\text{bf}} = 0$ and $S_{\text{bf}} = 1000$ provide the maximum (hereafter, Ni-max) and minimum (hereafter, Ni-min) limits on the NLTE effects in Ni lines, respectively. The former approach assumes no H-impact collisional ionization and the latter results in nearly thermalized (LTE) level populations. It has to be kept in mind, though, that the NLTE effects in Ni are very likely larger and thus, the O abundance might increase. We include the uncertainty related to the amplitude of NLTE effects in Ni into the final estimate of O abundance (Section 3.4).

Fig. 11 shows the line profiles of the 6300 Å and 5157.98 Å Ni I line, computed using the model atom with collisions scaled by $S_{\text{bf}} = 1000$ and $\log A(\text{Ni}) = 6.23$ dex. The latter spectral line was used in the analysis of the solar Ni abundance in Scott et al. (2015) and it appears to be relatively unblended compared to other Ni I features. Both lines are clearly weaker in 3D LTE compared to 1D LTE, and in 3D NLTE the difference is even larger. The weakening of Ni I lines in 3D LTE was also demonstrated by Scott et al. (2015),

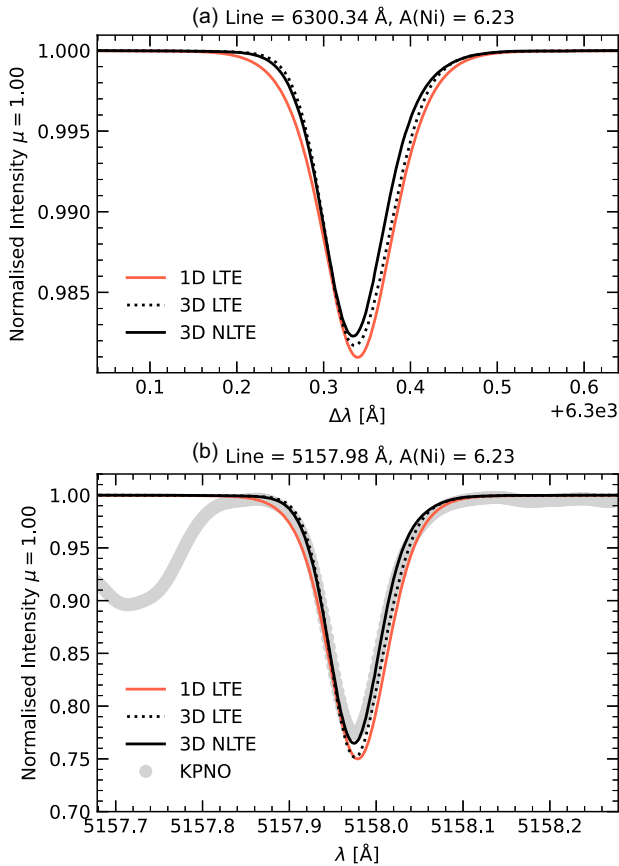


Figure 11. 1D LTE, 1D NLTE, and 3D NLTE line profiles of the Ni lines at 6300.34 Å (top panel) and 5157.98 Å (bottom panel). The 6300.34 Å feature blends with the forbidden O I line at 6300.304 Å.

although no NLTE calculations were performed in that study. To the best of our knowledge, Bruls (1993) and Vieytes & Fontenla (2013) are the only studies of NLTE effects Ni I in the solar spectrum, but they do not provide estimates of line EWs and NLTE abundance corrections in 1D and 3D, so a more quantitative comparison cannot be carried out.

Finally, we note that for Ni I, no quantum-mechanical estimates of photoionization cross-sections, H and e[−] collision rates are available. So we have to resort to classical recipes, but we caution that these recipes tend to underestimate the effects of overionization and line pumping, as detailed NLTE studies of other similar species demonstrated (e.g. Mn: Bergemann et al. 2019; Ti: Sitnova et al. 2020). Therefore our present calculations can be viewed as a conservative scenario, yet the actual NLTE effects in the Ni I lines are expected to be larger.

4.4 Centre-to-limb variation of oxygen abundances

We begin with the analysis of O abundances obtained for different μ angles and for different diagnostic lines of O. The best-fitting 3D NLTE and 1D LTE models are compared with the spatially resolved observations of the Sun in online Fig. A2.

Fig. 12 shows our abundance estimates obtained in 1D LTE, 1D NLTE, and 3D LTE for each of the five studied inclinations in the IAG and SST data (Section 2). Ideally, the slope α of the overdrawn trend line would equal zero, meaning that a given model returns self-consistent results at each angle. Low α values are therefore, to

a first order, a good indicator of a more reliable result. Additionally, online Fig. A4 (see the online Appendix) shows the observed EWs against the model predictions for 1D LTE, 1D NLTE, and 3D NLTE (LCAO+K). This figure is useful for its pedagogical content, to illustrate the failure of standard 1D or 3D LTE modelling. However, we do not use the actual observed EWs in the abundance analysis (see Section 4.6).

Clearly, the 1D LTE assumption does not yield reliable abundance estimates for the O I triplet (Fig. 12, top panels), as there is a strong negative correlation between the individual 1D LTE abundance estimates and the viewing angle, ranging from $\log A(\text{O}) \approx 8.8$ dex at the disc centre to $\log A(\text{O}) \approx 9.3$ dex at the limb ($\mu = 0.2$). Also the 3D LTE results are suboptimal: the slope is slightly smaller compared to 1D LTE, none the less the abundances range from $\log A(\text{O}) \approx 8.85$ dex at $\mu = 1$ to ≈ 9.10 dex at $\mu = 0.2$, with a significant systematic bias. 1D NLTE results are similar to 3D LTE in terms of the μ – $\log A(\text{O})$ slope, however, the disc-centre 1D NLTE abundance (here shown for the model atom LCAO+Kaul), $\log A(\text{O}) = 8.66$ dex, is in a much better agreement with the 3D NLTE disc-centre abundance obtained using the Stagger model, $\log A(\text{O}) = 8.70$ dex. However, the 3D NLTE approach clearly outperforms the analyses in that it leads to significantly stronger profiles of the triplet lines at the limb, thereby improving the agreement with the observations (see also Kiselman & Nordlund 1995; Asplund et al. 2004). The results obtained using the IAG and SST data are similar in terms of their CLV abundance slopes.

The forbidden [O I] line (Fig. 12, bottom panels) is less sensitive to the model atmosphere and to the O model atom, as the angle-dependent abundances are similar in 1D LTE and in 1D NLTE. However, all 3D NLTE and 3D LTE values are about 0.10 dex higher compared to 1D results. The differences between various 3D NLTE CLV results are entirely due to the differences in the predicted strength of the Ni blend at 6300.34 Å. The SST results show peculiar undulations, with abundances at $\mu = 1$ and $\mu = 0.4$ being significantly lower compared to other angles. The origin of this systematic is difficult to pin-point. It is possible that the subtraction of fringing and other instrumental artefacts in these data lead to residual systematic biases. In fact, it is clearly seen in fig. 2 of Pereira et al. (2009a) that the O I line unfortunately coincides with a minimum in the fringe pattern used to model the continuum of the SST data. The O abundances based on the IAG data at different angles are more internally consistent, supporting the choice of these observations as currently the most reliable data set.

4.5 Influence of O+H collisions

It is useful to look more closely into the abundances computed from different NLTE model atoms of O. In this respect, the most critical reactions are inelastic collisions between O and H atoms, which have a direct influence on the statistical equilibrium of O I.

As shown in Section 3.3, our new rate coefficients that describe the transitions in O I caused by collisions with H are different from the previous estimates by Barklem (2018). The latter quantities (LCAO) are on average smaller compared to the data computed using the QPC method. However, if we co-add the data from Barklem (2018) with the data from Kaulakys (1991), in order to account for the lack of short-rang interactions in the LCAO approach (as recommended by Amarsi et al. 2018), the net result is that for the majority of energy levels the combined LCAO+Kaulakys rates are higher compared to the LCAO and to the QPC data.

As a result, the O abundances computed from the 777 triplet lines using the three atomic models show a clear systematic difference

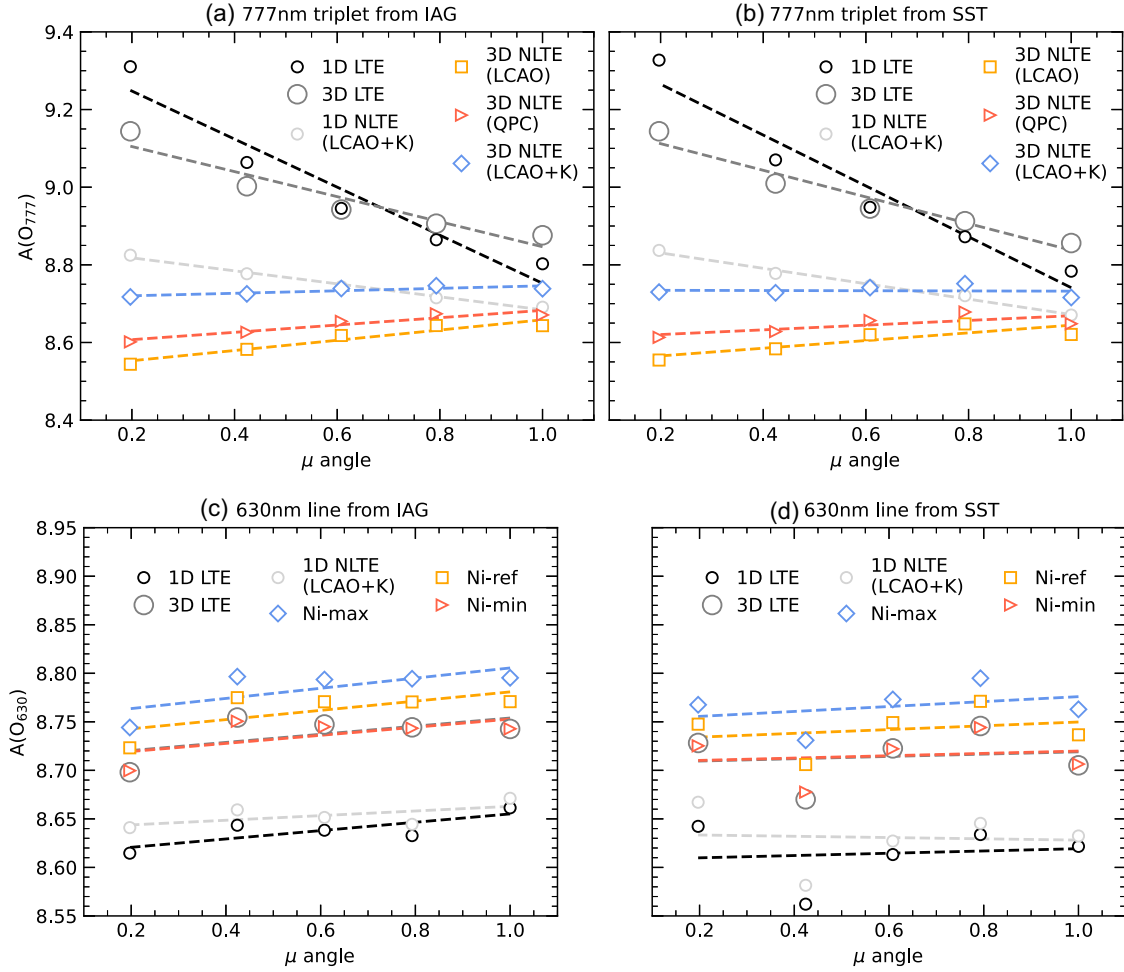


Figure 12. Centre-to-limb variation of the combined oxygen triplet for different model atom/atmosphere combinations. 1D is represented by the Marcs solar model and 3D is represented by the Stagger solar model.

(Fig. 12, top panels). The LCAO+Kaulakys model atom leads to a $\approx +0.1$ (disc centre) to $\approx +0.15$ dex (limb) higher solar O abundance compared to the LCAO and QPC models. This is because the latter two models, owing to the less efficient collisional thermalization they produce, yield larger NLTE effects in the 777 nm OI lines. However, neither of the atomic models can be given a preference, based on the CLV–abundance slope, because the moduli of the slopes are very similar. This suggests that the CLV of O lines alone is not sufficient as a metric to distinguish between the three NLTE atomic models. In other words, each of the model atoms – LCAO, QPC, or LCAO+Kaulakys – allows us to achieve internally consistent results, which are, however, systematically different with respect to each other.

For completeness, we note that the choice of collisional data in the O model atom is of no relevance in modelling the 630 nm oxygen line, as the populations of its energy levels are very close to thermal and the NLTE effects are very minor.

4.6 Model-data comparison

We determine the best-fitting abundances by employing the χ^2 statistics, comparing the observed data with the model line profiles. Line profiles for a fine grid of abundances are produced and for each observation we find the most probable abundance by minimising the

reduced χ^2 :

$$\chi^2 = \frac{1}{N_{\text{pix}} - N_{\text{free}}} \sum_i^{N_{\text{pix}}} \left[\frac{f_{\text{obs},i} - f_{\text{model},i}}{\sigma_{\text{obs},i}} \right]^2, \quad (1)$$

where N_{pix} is the number of wavelength points and N_{free} is 1 as the oxygen abundance is the only free parameter. The observational error $\sigma_{f_{\text{obs}}}$ represents the uncertainty caused by the limited S/N ratio of the data.

For the 777 nm triplet lines, we mask the observations to the region of $\pm 0.5 \text{ \AA}$ from the line centres and a few surrounding blends (Cr 1 at 7771.76 \AA , Ti 1 at 7771.41 \AA , Ti 1 at 7772.16 \AA , and Sc 1 7772.56 \AA), modelled in 1D LTE, are subtracted from the observations. These blends are weak and they are entirely contained in the absorption features associated with the triplet lines. Since the exact position of the line centres varies between different atlases and μ -angles, the models are slightly blue- or redshifted, so that the synthetic line centres match the observed data.

The 630 nm [OI] line is located in a region, which contains a number of blends, Si 1 (6299.599 \AA), Sc 2 (6300.698 \AA), and Fe 1 (6301.500 \AA). However, models are woefully inadequate to reproduce the observations in this region (online Fig. A5). So to estimate the contribution due to blends, that is to de-blend the O line, we adopted the following approach. We fitted arbitrary Voigt profiles to each of the blending features, allowing for the variation of

Table 5. Errors in O abundance calculations. The errors caused by the chromosphere and limited geometric resolution in 3D RT calculations are strictly systematic and they are directly applied to the resulting abundances. We note that these errors refer to the estimates at the disc centre. See the text.

Line Å	f -value (dex)	Ni blend (dex)	Observations (dex)	Chromosphere (dex)	Resolution (dex)
7771.940	± 0.026	–	± 0.015	+ 0.007	+ 0.010
7774.170	± 0.026	–	± 0.015	+ 0.007	+ 0.010
7775.390	± 0.026	–	± 0.015	+ 0.005	+ 0.010
6300.304	± 0.08	± 0.03	± 0.035	–0.003	+ 0.011

the amplitude, γ and σ parameters in the Gaussian and Lorentzian profiles. We also allowed for parabolic bisectors in order to deal with the asymmetry of both lines. This fit (online Fig. A6) was then used to determine the O abundance from the de-blended O+Ni feature using a mask with the width of ± 0.3 Å. The [O I] line was modelled using a grid of oxygen abundances, while the Ni was modelled with a fixed abundance of 6.23 dex. The meteoritic value has an uncertainty of 0.04 dex, but this uncertainty is entirely covered by the difference in the Ni blend contribution caused by adopting different NLTE atomic models of Ni.

4.7 Systematic errors

The model (systematic) error $\sigma_{f_{\text{model}}}$ comprises several sources, including the errors caused by the oscillator strengths and damping constants, as well as the errors associated with the limited geometric resolution of the 3D model atmosphere. These errors are not included in the χ^2 calculations (equation 1), but are considered separately in the abundance analysis (see Table 5).

4.7.1 Atomic data

The error caused by the uncertainty of oscillator strengths is fully correlated with the abundance error. As described in Section 3.1, we use the Hibbert et al. (1991) data for the 777 triplet lines and the Storey & Zeppen (2000) data for the 630 nm forbidden line. However, recently new f -values for allowed transitions were presented by Civiš et al. (2018). These data are based on the quantum defect theory (QDT) approach and, for the 777 nm triplet lines they are 12 per cent (-0.05 dex) lower than the f -values provided by Hibbert et al. (1991) and recommended by NIST. The difference between the f -values from the two sources is four times the NIST estimated uncertainty in the transition.

In order to understand the uncertainties of the f -values we carried out new atomic calculation. We used the code AUTOSTRUCTURE (Badnell 2011) to do multiple calculations of increasing complexity. We started with the same configuration expansion as used by Storey & Zeppen (2000). Further, we added additional configurations with the same orbitals with principal quantum number $n \leq 4$ and configurations with $n = 5$. In each case we tried different orbital optimization schemes. From the different calculations we find a scatter in the f -value of the 777 nm transitions of about 10 per cent with a tendency for the rate to be closer to lower value of Civiš et al. (2018) than to the Hibbert et al. (1991) value. Therefore, for the 777 lines we adopted the average of both values as our central value, and the associated f -value error (2σ) is assumed to be the difference between the both quantities.

The f -value for the magnetic dipole line at 630 nm is much more difficult to pin point. Such weak lines are generally very sensitive to

cancellation effects among different contributions from configuration interaction representations of the atomic levels. The main challenge is not the convergence of the expansion, but the sensitivity to how the orbitals are optimized. The NIST recommended transition probability for this line is $5.63 \times 10^{-3} \text{ s}^{-1}$ with the uncertainty flag B+ (better than 7 per cent), which is adopted from Baluja & Zeppen (1988) and Fischer & Saha (1983). The most recent calculations by Storey & Zeppen (2000) yield $6.45 \times 10^{-3} \text{ s}^{-1}$. This is a difference of ~ 15 per cent, which is more than twice the estimated uncertainty in this rate by NIST. The results of our own calculations show the rate varies widely between $\sim 3 \times 10^{-3} \text{ s}^{-1}$ and $\sim 1 \times 10^{-2} \text{ s}^{-1}$, with the best value being $\sim 8 \times 10^{-3} \text{ s}^{-1}$. As stated earlier, we use the Storey & Zeppen (2000) rate in our analysis, however, to account for the extreme sensitivity of the f -values to the details of orbital optimization, we assume a more realistic uncertainty of 20 per cent.

Finally, we investigated the uncertainty associated with damping, by performing spectrum synthesis calculations with a modified, by ± 10 per cent, value of the damping constant. This, however, has a negligible influence on the O triplet and [O I] lines and is therefore neglected.

4.7.2 Geometric resolution

We also take into account a systematic error associated with the limited geometric resolution of 3D model atmospheres used in radiative transfer calculations. This correction is estimated as follows. The two families of photospheric 3D atmospheres employed in this paper have (x,y,z) -resolutions of $240 \times 240 \times 230$ (STAGGER) and $512 \times 512 \times 192$ (Bifrost-phot). We restrain from re-sampling the vertical resolution, but down-sample the number of vertical columns, ensuring that we have enough columns to maintain the ratio of intergranular lanes to granules covering the entire simulation. We converted a single STAGGER snapshot to horizontal resolutions 5×5 , 10×10 , 20×20 , 30×30 , and 120×120 and computed equivalent widths of the diagnostic O I lines for each down-sampled snapshot. Similarly, equivalent widths for a photospheric Bifrost snapshot with different horizontal resolutions between 10×10 and 160×160 were computed. These calculations were carried out in LTE, because our previous analysis (Bergemann et al. 2019) confirmed that the scaling is very similar in LTE and in NLTE. We find that the horizontal resolution of $(x, y) = (30, 30)$ offers a reasonable compromise between the computational expense of 3D NLTE modelling and the physical realism, leading to a small (~ 1 – 2 per cent) systematic error in the line strength compared to that obtained the full geometric setup. To correct for this small bias, we extract the geometric resolution correction (Table 5) by comparing the EWs of lines computed at our nominal resolution and at the highest-possible resolution. This correction is then separately applied to the abundance determined at each μ angle. The results are shown in Fig. 13. The disc centre and limb results are not very sensitive to this effect, but at $\mu = 0.8$ and $\mu = 0.6$, the EW error caused by using the horizontal resolution of $(x, y) = (30, 30)$ can be as large as 3 per cent. For the disc centre, the abundance correction for the diagnostic O lines amounts to 0.01 dex.

4.7.3 Influence of the chromosphere

We do not use the Bifrost models to derive the absolute solar O abundance (Section 3.5), but only to quantify the influence of the chromosphere, that is, the re-adjustment of the photospheric structure under the influence of the chromosphere, on the line formation

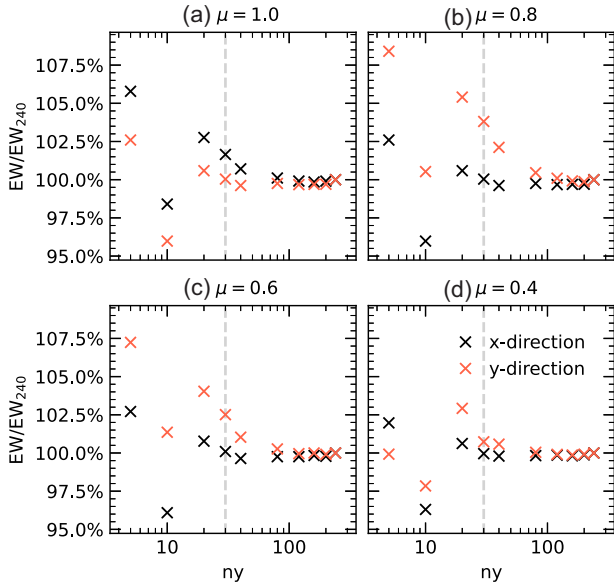


Figure 13. Influence of the geometrical resolution (nx, ny) of 3D STAGGER model on the measured equivalent widths. Here nx is kept constant at 5. ny varies from 5 to 240, where 240×240 corresponds to the full resolution of the model. The vertical dashed line shows our default geometric resolution (30,30) adopted in 3D NLTE radiative transfer calculations.

Table 6. Final 3D NLTE abundance estimates obtained from the 777 and 630 nm oxygen lines.

	777 nm	630 nm
IAG	8.739	8.771
SST	8.716	8.737
Hinode	–	8.748
DST	–	8.799

and on the O abundances. This is done by comparing the results calculated with two types of *Bifrost* models: (a) the full simulation covering the photosphere and the chromosphere, and (b) the strictly photospheric simulation (Section 3.5). Each simulation represents an extended time series, from which we extract 10 snapshots for the detailed radiative transfer. The average difference between the T_{eff} values of the snapshots is 10 K.

Comparing the O abundances derived using the two *Bifrost* model sequences in 3D NLTE, we find that the abundance differences are not large (Table 5). The chromosphere weakens the 777 triplet lines that corresponds to the increase of O abundance by $\sim +0.01$ dex at the disc centre and $+0.02$ dex at the limb relative to a pure photospheric simulation. The 6300 [O I] line is relatively unaffected by the chromosphere, and the O abundance inferred from this line is only 0.003 dex lower. We note that even ignoring the snapshot with the largest T_{eff} difference (16 K) does not alter the estimate of chromospheric correction by more than 0.001 dex.

Whereas the chromospheric correction for the O lines is small, the presence of a chromosphere may have a larger influence on the spectral lines that form higher up in the layers close and above the temperature minimum, such as the Ni 6767 Å helioseismology line.

4.8 Final O abundance

Table 6 provides our estimates of the photospheric O abundance computed in 3D NLTE from different observational data sets, where

the results were corrected for the chromospheric and spatial resolution effects (Sections 4.7.2, 4.7.3). The individual results obtained in 1D LTE, 1D NLTE, 3D NLTE with different atomic models are provided in online Table A1 (see the online Appendix). The EWs of the corresponding lines are tabulated in online Table A2 (see the online Appendix).

To compute the final estimates of O abundance and its uncertainties from different observational data and different atomic models, we proceed as follows. For both 777 and 630 nm lines, we adopt the central values as derived from the IAG data using the LCAO+K model atom of O, because of the superior resolving power of these observations and more consistent estimates of abundances derived from the spatially resolved spectra taken at different pointings across the solar disc.⁸ The LCAO+K (with Kaulakys data) atomic model, furthermore, provides a flatter CLV abundance slope, compared to the LCAO or QPC collisional data, but also from the perspective of atomic physics, the Kaulakys data appear to be necessary, as they are expected to compensate for the lack of short-range interactions in the quantum-mechanical calculations. We also adopt the $S_{\text{bf}} = 100$ model atom of Ni, as this NLTE model provides the average of the plausible 3D NLTE Ni blend contributions to the [O I] feature that corresponds to the average between the extremely high, moderate, and negligible collision rates (Section 4.3).

To estimate the final combined uncertainties, we resort to a Monte Carlo simulation and make use of the central limit theorem, which states that the normalized sum of random uncorrelated variables closely follows a normal distribution, regardless of the shape of the distribution function of individual variables. This is a commonly used approach in case when the shapes of uncertainties are not known, as in our case. The errors associated with the analysis (see Table 5) are used to generate three uniform distributions (large samples of 1 million points each), representing (a) the uncertainty of the oscillator strengths (f -value), (b) the uncertainty caused by the Ni blend (630 nm line) and that caused by the O+H collisional data (777 nm lines), and (c) the uncertainty caused by using different observed spectra. The uncertainty caused by the collisional data is taken to be the difference between the QPC and LCAO+K results. The latter is assumed to be one half of the difference between the SST (min) and the IAG (max) results for the 777 nm line, and that between the SST (min) and DST (max) results for the 630 nm line. These errors are co-added and one standard deviation (1σ) of the resulting distribution (Fig. 14) is adopted as the final uncertainty. We note that the final combined distribution of errors for the 777 nm line is very close to normal, whereas for the 630 nm line there is a small deviation owing to a large dominant uncertainty source. However, this has no influence on the conclusions.

As a result, our 3D NLTE value derived from the 777 and 630 nm lines is $\log A(\text{O}) = 8.739 \pm 0.027$ dex and $\log A(\text{O}) = 8.771 \pm 0.053$ dex, respectively. Assuming that the results are independent, we can combine them to obtain the final photospheric O abundance value of $\log A(\text{O}) = 8.75 \pm 0.03$ dex.

We note that if we were to use the old Hibbert et al. (1991) f -values and the SST data, our results based on the LCAO+K model atom of O would be in excellent agreement with the 3D NLTE estimate by Amarsi et al. (2018) who relied on the same input. Likewise, our 1D NLTE result based on the MARCS model is in agreement with that by Sitnova & Mashonkina (2018).

⁸We note that no optimization by hand was involved in the analysis.

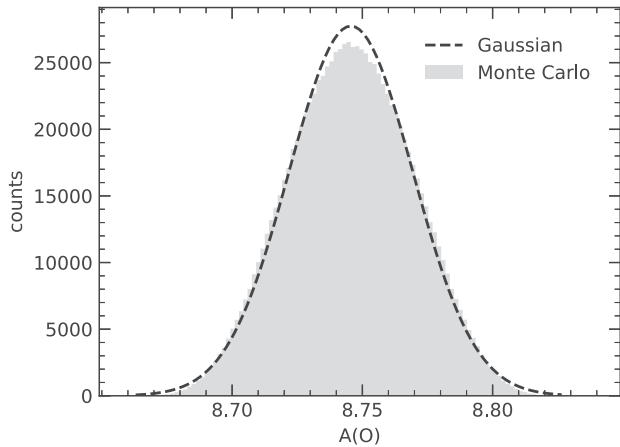


Figure 14. Final combined distribution function for the solar photospheric abundance of oxygen. See Section 4.8. A normal distribution is overlotted with a thin line, for comparison.

5 DISCUSSION

Our estimates of O abundances based on the permitted 777 nm triplet lines and on the 630 forbidden [O I] line are in a good agreement within the respective uncertainties. The triplet lines are, however, sensitive to the input physics of the O model atom, whereas the forbidden line is sensitive to the input physics of the Ni model atom, primarily to the collisional data. Also, the f -values carry a significant source of uncertainty, as the direct experimental verification of the transition probabilities for the 777 and 630 nm is not possible. These errors are associated with the physical limitations of theory of atomic physics, molecular physics, and collisional dynamics, and, therefore, their true distributions are unknown. Nonetheless, considering all sources of error, it is very plausible that the photospheric O abundance is close to $\log A(\text{O}) = 8.75$ dex.

It is interesting to discuss our results in comparison with the other recent estimates of the solar photospheric O abundance. Amarsi et al. (2018) and Asplund, Amarsi & Grevesse (2021) found $\log A(\text{O}) = 8.69 \pm 0.03$ dex and 8.69 ± 0.04 dex, respectively. The former estimate is based on the 777 nm line, while the latter also includes the 630 nm and selected molecular OH lines. In principle, our results and those by this group are not inconsistent within their combined uncertainties. Our value is in a much better agreement with the values proposed by Caffau et al. (2008), Caffau et al. (2015), and Steffen et al. (2015), who analysed different O lines, including several forbidden [O I] lines, the 777 triplet, and the near-IR O I features. Another recent study of the solar photospheric O abundance is that by Cubas Armas, Asensio Ramos & Socas-Navarro (2020). Their analysis is based on a semi-empirical method of determining the abundance by inverting spatially resolved observed solar spectra. Their estimate, based on the forbidden [O I] line at 630 nm, is $\log A(\text{O}) = 8.80 \pm 0.03$ dex, also consistent with our results for this feature.

6 CONCLUSIONS

We present a re-analysis of the solar photospheric O abundance using new atomic data for O and different 3D radiation hydrodynamical models of solar atmospheres. The NLTE model atom includes novel rates of collisions between O and H atoms, computed

using the quantum hopping probability current method (Belyaev et al. 2019), increasing the number of O I terms with accurate collisional data to 16. The R-matrix method for atomic scattering calculations (Berrington et al. 1978) is employed to compute new photoionization cross-sections and the rates describing transitions caused by inelastic processes in collisions of O atoms with free electrons. We also present a new comprehensive model atom of Ni, which, for the lack of detailed quantum-mechanical data, is still based on classical formulae for photoionization and collisional reaction rates. We use the 1D MARCS solar model atmosphere, the 3D Stagger model (Collet et al. 2011; Magic et al. 2013), and two versions of 3D MHD models computed self-consistently, with and without the chromosphere, using the Bifrost code (Carlsson et al. 2016).

The model atoms are used to perform 1D LTE, 1D NLTE, and 3D NLTE radiative transfer calculations and abundance analysis of O lines in the solar spectrum. We focus on the least blended lines of O I at 7771, 7774, 7775 Å, and we also consider the forbidden O I line at 6300 Å. We also perform 3D NLTE calculations of the Ni I blend at 6300.341 Å, which contributes about 25 per cent of the entire absorption feature. The observational data are taken from different sources. Our primary source of data are the new spatially resolved spectra taken with the IAG FTS instrument. The data have a resolving power of $R \sim 700\,000$, much higher compared to all previously available solar data. Similar to previous studies, we also include the spectra obtained with the ground-based Swedish Solar Telescope (Pereira et al. 2009a), the DST (Takeda & UeNo 2019), and with the space-based Solar Optical Telescope on the *Hinode* satellite (Caffau et al. 2015).

We obtain the solar O abundance of $\log A(\text{O}) = 8.739 \pm 0.027$ dex and $\log A(\text{O}) = 8.771 \pm 0.053$ dex based on the 777 nm triplet and 630 nm forbidden [O I] lines, respectively. Our final combined value is $\log A(\text{O}) = 8.75 \pm 0.03$ dex, which is close to the estimate proposed in the compilation of the solar abundances by Caffau et al. (2008, 8.76 ± 0.07 dex), but slightly higher than the recent value by Asplund et al. (2021, 8.69 ± 0.04 dex). The differences between our and previous results can be explained by the updated transition probabilities for the 777 lines, new higher-resolution observations collected with the IAG FTS facility, 3D NLTE modelling of the Ni blend, and a correction for a systematic bias caused by the chromospheric back-heating. These effects add up to increase the solar abundance by about +0.05 dex relative to the value proposed by Asplund et al. In addition, we confirm that using the HINODE space-based data, which were employed by Caffau et al. (2015), we recover a slightly higher abundance compared to the value obtained by using the SST data chosen by Asplund et al. (2021).

Our results thus suggest that the question of whether the solar photospheric O abundance is low or high, that is closer to the values from Grevesse & Sauval (1998), is still open. There are remaining controversies associated with modelling of the permitted 777 nm lines and of the forbidden [O I] line. First, the large systematic differences between two sources of H-impact collisional data (Kaulakys 1991 and Belyaev et al. 2019) must be resolved. Second, the differences between the new lower f -values from Civiš et al. (2018) and the older values from Hibbert et al. (1991) must be settled. Until then, we recommend to use the average of the values from both sources. Our results suggest that the indirect influence of the chromosphere on the O lines in the solar spectrum is not large. However, it is desirable to perform new self-consistent 3D R(M)HD simulations of the solar atmosphere, including chromosphere, with the state-of-the-art microphysics and NLTE radiative transfer.

ACKNOWLEDGEMENTS

We are grateful to the anonymous referee for the helpful remarks and suggestions on the manuscript. We thank Elisabetta Caffau for providing the spectra taken with Solar Optical Telescope on the *Hinode* satellite. We are grateful to Martin Asplund and Hans-Guenther Ludwig for valuable discussions and comments on the manuscript. SAY, YVV, and AKB gratefully acknowledge support from the Ministry of Education (the Russian Federation), project FSZN-2020-0026. MB and ES are supported through the Lise Meitner grant from the Max Planck Society. We acknowledge support by the Collaborative Research Centre SFB 881 (projects A5, A10), Heidelberg University, of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation). ME is supported through the SPP 1992 *Exoplanet Diversity* grant RE 1664/17-1.

DATA AVAILABILITY

The O model atoms (QPC, LCAO, LCAO+K) and the error map representing the blends around the 630.0 nm O+Ni feature are available at <https://keeper.mpg.de/d/da74c98c1c9c4477b67f/>.

REFERENCES

- Acton C. H., 1996, *Planet. Space Sci.*, 44, 65
- Allende Prieto C., Lambert D. L., Asplund M., 2001, *ApJ*, 556, L63
- Amarsi A. M., Barklem P. S., Asplund M., Collet R., Zatsarinny O., 2018, *A&A*, 616, A89
- Asplund M., Grevesse N., Sauval A. J., Allende Prieto C., Kiselman D., 2004, *A&A*, 417, 751
- Asplund M., Grevesse N., Sauval A. J., Scott P., 2009, *ARA&A*, 47, 481
- Asplund M., Amarsi A. M., Grevesse N., 2021, preprint ([arXiv:2105.01661](https://arxiv.org/abs/2105.01661))
- Badnell N. R., 1997, *J. Phys. B: At. Mol. Phys.*, 30, 1
- Badnell N. R., 2011, *Comput. Phys. Commun.*, 182, 1528
- Bahcall J. N., Serenelli A. M., Basu S., 2005, *ApJ*, 621, L85
- Bailey J. E. et al., 2015, *Nature*, 517, 56
- Baluja K. L., Zeppen C. J., 1988, *J. Phys. B: At. Mol. Phys.*, 21, 1455
- Barbuy B., Chiappini C., Gerhard O., 2018, *ARA&A*, 56, 223
- Barklem P. S., 2007, *A&A*, 462, 781
- Barklem P. S., 2016, *A&AR*, 24, 9
- Barklem P. S., 2018, *A&A*, 610, A57
- Barklem P. S., Piskunov N., O'Mara B. J., 2000, *A&AS*, 142, 467
- Bedell M., Meléndez J., Bean J. L., Ramírez I., Leite P., Asplund M., 2014, *ApJ*, 795, 23
- Bedell M. et al., 2018, *ApJ*, 865, 68
- Belyaev A. K., 1993, *Phys. Rev. A*, 48, 4299
- Belyaev A. K., 2013, *Phys. Rev. A*, 88, 052704
- Belyaev A. K., Yakovleva S. A., 2017, *A&A*, 606, A147
- Belyaev A. K., Voronov Y. V., Mitrushchenkov A., Guitou M., Feautrier N., 2019, *MNRAS*, 487, 5097
- Bergemann M., Nordlander T., 2014, preprint ([arXiv:1403.3088](https://arxiv.org/abs/1403.3088))
- Bergemann M., Lind K., Collet R., Magic Z., Asplund M., 2012, *MNRAS*, 427, 27
- Bergemann M. et al., 2019, *A&A*, 631, A80
- Berrington K. A., Burke P. G., Le Dourneuf M., Robb W. D., Taylor K. T., Ky Lan V., 1978, *Comput. Phys. Commun.*, 14, 367
- Berrington K. A., Eissner W. B., Norrington P. H., 1995, *Comput. Phys. Commun.*, 92, 290
- Bochsler P., 2007, *A&A*, 471, 315
- Braut J., 1972, Kitt Peak solar atlas. Kitt Peak Observatory, Tucson
- Bruils J. H. M. J., 1993, *A&A*, 269, 509
- Buchhave L. A., Latham D. W., 2015, *ApJ*, 808, 187
- Caffau E., Ludwig H. G., Steffen M., Ayres T. R., Bonifacio P., Cayrel R., Freytag B., Plez B., 2008, *A&A*, 488, 1031
- Caffau E., Ludwig H. G., Steffen M., Livingston W., Bonifacio P., Malherbe J. M., Doerr H. P., Schmidt W., 2015, *A&A*, 579, A88
- Carlsson M., 1992, in Giampapa M. S., Bookbinder J. A., eds, ASP Conf. Ser. Vol. 26, Cool Stars, Stellar Systems, and the Sun. Astron. Soc. Pac., San Francisco, p. 499
- Carlsson M., Hansteen V. H., Gudiksen B. V., Leenaarts J., De Pontieu B., 2016, *A&A*, 585, A4
- Civiš S., Kubelík P., Ferus M., Zanozina E. M., Pastorek A., Naskidashvili A. V., Chernov V. E., 2018, *ApJS*, 239, 11
- Collet R., Magic Z., Asplund M., 2011, *J. Phys. Conf. Ser.*, 328, 012003
- Cubas Armas M., Asensio Ramos A., Socas-Navarro H., 2020, *A&A*, 643, A142
- Cunto W., Mendoza C., 1992, *Rev. Mex. Astron. Astrofis.*, 23, 107
- Ding M. D., Qiu J., Wang H., 2002, *ApJ*, 576, L83
- Doerr H. P., 2015, PhD thesis, Univ. Freiburg
- Drawin H.-W., 1968, *Z. Phys.*, 211, 404
- Fischer C. F., Saha H. P., 1983, *Phys. Rev. A*, 28, 3169
- Gallagher A. J., Bergemann M., Collet R., Plez B., Leenaarts J., Carlsson M., Yakovleva S. A., Belyaev A. K., 2020, *A&A*, 634, A55
- Grevesse N., Sauval A. J., 1998, *Space Sci. Rev.*, 85, 161
- Gudiksen B. V., Carlsson M., Hansteen V. H., Hayek W., Leenaarts J., Martínez-Sykora J., 2011, *A&A*, 531, A154
- Gustafsson B., 1973, *Uppsala Astron. Obs. Ann.*, 5, 1
- Gustafsson B., Bell R. A., Eriksson K., Nordlund A., 1975, *A&A*, 500, 67
- Hibbert A., Biemont E., Godefroid M., Vaecck N., 1991, *J. Phys. B: At. Mol. Phys.*, 24, 3943
- Johansson S., Litzén U., Lundberg H., Zhang Z., 2003, *ApJ*, 584, L107
- Kaulakys B., 1985, *J. Phys. B: At. Mol. Phys.*, 18, L167
- Kaulakys B., 1991, *J. Phys. B: At. Mol. Phys.*, 24, L127
- Kewley L. J., Ellison S. L., 2008, *ApJ*, 681, 1183
- Kiselman D., 1991, *A&A*, 245, L9
- Kiselman D., Nordlund A., 1995, *A&A*, 302, 578
- Kramida A., Yu. Ralchenko Reader J., NIST ASD Team, 2020, NIST Atomic Spectra Database (ver. 5.8). National Institute of Standards and Technology, Gaithersburg, MD [Online]. Available: <https://physics.nist.gov/asd>
- Kunasz P., Auer L. H., 1988, *J. Quant. Spectrosc. Radiat. Transfer*, 39, 67
- Laming J. M. et al., 2017, *ApJ*, 851, L12
- Leenaarts J., Carlsson M., 2009, in Lites B., Cheung M., Magara T., Mariska J., Reeves K., eds, ASP Conf. Ser. Vol. 415, The Second *Hinode* Science Meeting: Beyond Discovery-Toward Understanding. Astron. Soc. Pac., San Francisco, p. 87
- Leenaarts J., Carlsson M., Rouppe van der Voort L., 2012, *ApJ*, 749, 136
- Litzén U., Braut J. W., Thorne A. P., 1993, *Phys. Scr.*, 47, 628
- Lodders K., 2003, *ApJ*, 591, 1220
- Lorenzo-Oliveira D. et al., 2018, *A&A*, 619, A73
- Magic Z. et al., 2013, *A&A*, 557, A26
- Mihalas D., Dappen W., Hummer D. G., 1988, *ApJ*, 331, 815
- Mitrushchenkov A., Guitou M., Belyaev A. K., Voronov Y. V., Feautrier N., 2019, *J. Chem. Phys.*, 150, 064312
- Moustakas J., Kennicutt Robert C. J., Tremonti C. A., Dale D. A., Smith J.-D. T., Calzetti D., 2010, *ApJS*, 190, 233
- Nagayama T. et al., 2019, *Phys. Rev. Lett.*, 122, 235001
- Neckel H., Labs D., 1984, *Sol. Phys.*, 90, 205
- Nemer A. et al., 2019, *ApJ*, 887, L9
- Nissen P. E., Christensen-Dalsgaard J., Mosumgaard J. R., Silva Aguirre V., Spitoni E., Verma K., 2020, *A&A*, 640, A81
- Nordlund Å., Galsgaard K., 1995, Technical Report: A 3D MHD Code for Parallel Computers. Niels Bohr Institute, Univ. Copenhagen. Available at: http://www.astro.ku.dk/~kg/Papers/MHD_code.ps.gz
- Nordlund Å., Stein R. F., Asplund M., 2009, *Living Rev. Sol. Phys.*, 6, 2
- Osorio Y., Barklem P. S., Lind K., Belyaev A. K., Spielfiedel A., Guitou M., Feautrier N., 2015, *A&A*, 579, A53
- Pereira T. M. D., Kiselman D., Asplund M., 2009a, *A&A*, 507, 417
- Pereira T. M. D., Asplund M., Kiselman D., 2009b, *A&A*, 508, 1403
- Pinsonneault M. H., Delahaye F., 2009, *ApJ*, 704, 1174
- Rees M. H., 1989, *Physics and Chemistry of the Upper Atmosphere*. Cambridge Univ. Press, Cambridge

- Reiners A., Mrotzek N., Lemke U., Hinrichs J., Reinsch K., 2016, *A&A*, 587, A65
- Rybicki G. B., Hummer D. G., 1991, *A&A*, 245, 171
- Rybicki G. B., Hummer D. G., 1992, *A&A*, 262, 209
- Schäfer S., Royen K., Zapke A. H., Ellwarth M., Reiners A., 2020, in Evans C. J., Bryant J. J., Motohara K., eds, Proc SPIE Conf. Ser. Vol. 11447, Ground-based and Airborne Instrumentation for Astronomy VIII. SPIE, Bellingham, p. 2187
- Scharmer G. B., Bjelksjo K., Korhonen T. K., Lindberg B., Petterson B., 2003, in Keil S. L., Avakyan S. V., eds, Proc. SPIE Conf. Ser. Vol. 4853, Innovative Telescopes and Instrumentation for Solar Astrophysics. SPIE, Bellingham, p. 341
- Scott P., Asplund M., Grevesse N., Bergemann M., Sauval A. J., 2015, *A&A*, 573, A26
- Seaton M. J., 1962, in Bates D. R., ed., Atomic and Molecular Processes. Academic Press, New York, p. 375
- Serenelli A. M., Basu S., Ferguson J. W., Asplund M., 2009, *ApJ*, 705, L123
- Sitnova T. M., Mashonkina L. I., 2018, *Astron. Lett.*, 44, 411
- Sitnova T. M., Mashonkina L. I., Ryabchikova T. A., 2013, *Astron. Lett.*, 39, 126
- Sitnova T. M., Yakovleva S. A., Belyaev A. K., Mashonkina L. I., 2020, *Astron. Lett.*, 46, 120
- Slanger T. G. et al., 2011, *EOS, Trans. Am. geophys. Un.*, 92, 291
- Snodgrass H. B., Ulrich R. K., 1990, *ApJ*, 351, 309
- Socas-Navarro H., 2015, *A&A*, 577, A25
- Steffen M., Prakapavičius D., Caffau E., Ludwig H. G., Bonifacio P., Cayrel R., Kučinskas A., Livingston W. C., 2015, *A&A*, 583, A57
- Storey P. J., Zeippen C. J., 2000, *MNRAS*, 312, 813
- Takeda Y., UeNo S., 2019, *Sol. Phys.*, 294, 63
- Tolstoy E., Hill V., Tosi M., 2009, *ARA&A*, 47, 371
- Unsöld A., 1955, Physik der Sternatmosphären mit besonderer Berücksichtigung der Sonne. Springer-Verlag, Berlin
- van Regemorter H., 1962, *ApJ*, 136, 906
- Vieytes M. C., Fontenla J. M., 2013, *ApJ*, 769, 103
- Villante F. L., Serenelli A., 2020, preprint ([arXiv:2004.06365](https://arxiv.org/abs/2004.06365))
- Vincent A. C., Scott P., Serenelli A., 2015, *Phys. Rev. Lett.*, 114, 081302
- Wood M. P., Lawler J. E., Sneden C., Cowan J. J., 2014, *ApJS*, 211, 20

SUPPORTING INFORMATION

Supplementary data are available at *MNRAS* online.

bergemann_suppl_material

Please note: Oxford University Press is not responsible for the content or functionality of any supporting materials supplied by the authors. Any queries (other than missing material) should be directed to the corresponding author for the article.

This paper has been typeset from a $\text{\TeX}/\text{\LaTeX}$ file prepared by the author.